WRF/Chem Version 3.5 User's Guide

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DISCLAIMERS

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WRF-Chem Version 3.5 User's Guide

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WRF-Chem Overview

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1.1 Introduction

The WRF-Chem User's Guide is designed to provide the reader with information specific to the chemistry part of the WRF model and its potential applications. It will provide the user a description of the WRF-Chem model and discuss specific issues related to generating a forecast that includes chemical constituents beyond what is typically used by today's meteorological forecast models. For additional information regarding the WRF model, the reader is referred to the WRF model User's Guide (http://www.mmm.ucar.edu/wrf/users/docs/user_guide_V33/contents.html).

Presently, the WRF-Chem model is now released as part of the Weather Research and Forecasting (WRF) modeling package. And due to this dependence upon WRF, it is assumed that anyone choosing to use WRF-Chem is very familiar with the set-up and use of the basic WRF model. It would be best for new WRF users to first gain training and experience in editing, compiling, configuring, and using WRF before venturing into the more advanced realm of setting up and running the WRF-Chem model.

The WRF-Chem model package consists of the following components (in addition to resolved and non-resolved transport) as well as some additional unlisted capabilities:

- Dry deposition, coupled with the soil/vegetation scheme
- Four choices for biogenic emissions:
  - No biogenic emissions included
  - Online calculation of biogenic emissions as in Simpson et al. (1995) and Guenther et al. (1994) includes emissions of isoprene, monoterpenes, and nitrogen emissions by soil
  - Online modification of user-specified biogenic emissions - such as the EPA Biogenic Emissions Inventory System (BEIS) version 3.14. The user must provide the emissions data for their own domain in the proper WRF data file format
  - Online calculation of biogenic emissions from MEGAN
- Three choices for anthropogenic emissions:

- No anthropogenic emissions
- Global emissions data from the one-half degree RETRO and ten-degree EDGAR data sets
- User-specified anthropogenic emissions such as those available from the U.S. EPA NEI-05 data inventory. The user must provide the emissions data for their own domain in the proper WRF data file format

- Several choices for gas-phase chemical mechanisms including:
  - RADM2, RACM, CB-4 and CBM-Z chemical mechanisms
  - The use of the Kinetic Pre-Processor, (KPP) to generate the chemical mechanisms. The equation files (using Rosenbrock type solvers) are currently available for RADM2, RACM, RACM-MIM, SAPRC-99, MOZART and NMHC9 chemical mechanisms
- Three choices for photolysis schemes:
  - Madronich scheme coupled with hydrometeors, aerosols, and convective parameterizations. This is a computationally intensive choice, tested with many setups
  - Fast-J photolysis scheme coupled with hydrometeors, aerosols, and convective parameterizations
  - F-TUV photolysis scheme. This scheme, also from Sasha Madronich, is faster than the previous Madronich scheme option.
- Five choices for aerosol schemes:
  - The Modal Aerosol Dynamics Model for Europe - MADE/SORGAM
  - The Modal Aerosol Dynamics Model for Europe with the Volitity Basis Set aerosols – MADE/VBS
  - The Modal Aerosol Module (MAM) 3 or 7 bin schemes closely coupled to the CAM5 physics
  - The Model for Simulating Aerosol Interactions and Chemistry (MOSAIC - 4 or 8 bins) sectional model aerosol parameterization
  - A bulk aerosol module from GOCART
- Aerosol direct effect through interaction with atmospheric radiation, photolysis, and microphysics routines. In version 3.5 this is available for all aerosol options
- Aerosol indirect effect through interaction with atmospheric radiation, photolysis, and microphysics routines. In V3.5 this option is available for modal and sectional aerosol options
- An option for the passive tracer transport of greenhouse gases
- Two options for a 10-bin volcanic ash aerosol scheme based upon emissions from a single active volcano. One scheme includes SO_2 degassing from the volcano while the other ignores SO_2 degassing. Volcanic ash emissions can also be coupled to some aerosol modules (bulk and modal)
- A tracer transport option in which the chemical mechanism, deposition, etc. has been turned off. The user must provide the emissions data for their own domain in the proper WRF data file format for this option. May be run parallel with chemistry
- A plume rise model to treat the emissions of wildfires

1.2 WRF-Chem software

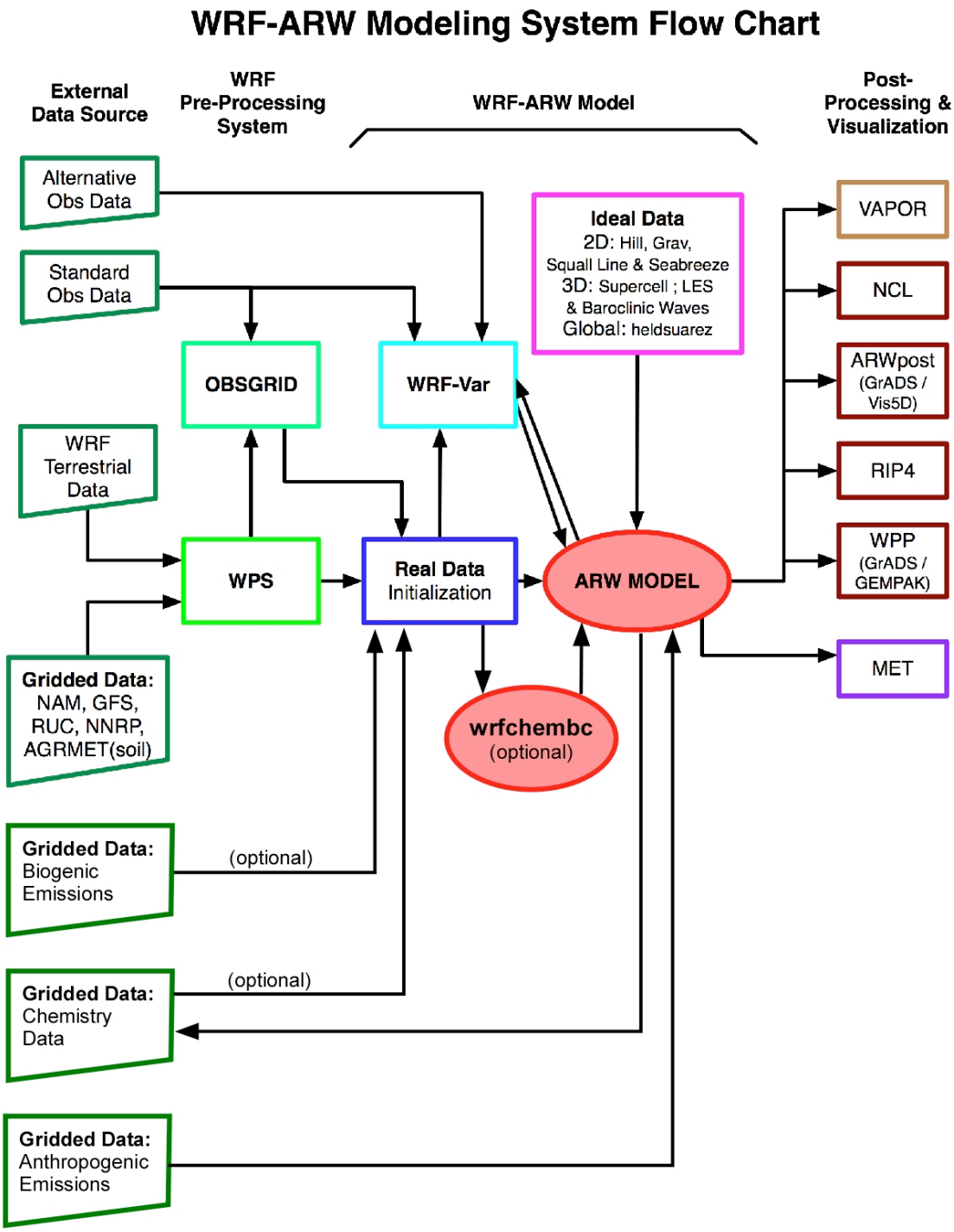
The chemistry model has been built to be consistent with the WRF model I/O Applications Program Interface (I/O API). That is, the chemistry model section has been built following the construction methodology used in the remainder of the WRF model. Therefore, the reader is referred to the WRF software description in the WRF User's Guide (Chapter 7) for additional information regarding software features like the build mechanism and adding arrays to the WRF registry. And while the chemistry model has been built with the intent to work within the WRF framework, *not all run time options (e.g., physical parameterizations) that are available for WRF will function properly with chemistry turned on*. Therefore, care must be taken in selecting the parameterizations used with the chemistry schemes.

1.3 Possible applications of the current modeling system

- Prediction and simulation of weather, or regional and local climate
- Coupled weather prediction/dispersion model to simulate release and transport of constituents
- Coupled weather/dispersion/air quality model with full interaction of chemical species with prediction of O_3 and UV radiation as well as particulate matter (PM)
- Study of processes that are important for global climate change issues. These include, but are not restricted to the aerosol direct and indirect forcing

1.4 The WRF-Chem modeling system overview

The following figure shows the flowchart for the WRF-Chem modeling system version 3.5.



As shown in the diagram, the WRF-Chem modeling system follows the same structure as the WRF model by consisting of these major programs:

- The WRF Pre-Processing System (WPS)
- WRF-Var data assimilation system

- WRF solver (ARW core only) including chemistry

- Post-processing and visualization tools

The difference with regular WRF comes from the chemistry part of the model needing to be provided additional gridded input data related to emissions. This additional input data is provided either by the WPS (dust emission fields), or read in during the real.exe initialization (e.g., biomass burning, biogenic emissions, GOCART background fields, etc.), or read in during the execution of the WRF solver (e.g., anthropogenic emissions, boundary conditions, volcanic emissions, etc.). And while some programs are provided in an attempt to aid the user in generation of these external input data files, as stated earlier, not all emissions choices are set-up to function for all possible namelist options related to the WRF-Chem model. In other words, the generation of emissions input data for simulating the state of the atmosphere's chemistry can be incredibly complex. Some times the user will need to modify code, or the model configuration, to get it to function properly for their project.

Chapter 2: WRF-Chem Software Installation

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2.1 Introduction

The WRF modeling system software (including chemistry) installation is straightforward on the ported platforms. The package is mostly self-contained, meaning that WRF requires no external libraries that are not already supplied with the code. One exception for WRF is the netCDF library, which is one of the supported I/O API packages. The netCDF libraries or source code are available from the Unidata homepage at http://www.unidata.ucar.edu (select the pull-down tab Downloads, registration required, to find the netCDF link). Likewise, there is one exception as well, the fast lexical analyser (FLEX) library (libfl.a) will be needed if compiling the KPP chemistry code. This library is commonly included with GNU bison and is freely available for download at http://www.gnu.org/software/bison if it is not already installed on your unix systm.

The WRF-Chem model has been successfully ported to a number of Unix-based machines. We do not have access to all tested systems and must rely on outside users and vendors to supply required configuration information for compiler and loader options of computing architectures that are not available to us. See also chapter 2 of the User's Guide for the Advanced Research WRF for a list of the supported combinations of hardware and software, required compilers, and scripting languages as well as post-processing software. It cannot be guaranteed that chemistry will build successfully on all architectures that have been tested for the meteorological version of WRF.

Note that this document assumes *a priori* that the reader is very familiar with the installation and implementation of the WRF model and its initialization package (e.g., the WRF Preprocessing System, or WPS). Documentation for the WRF Model and its initialization package can be found at (http://www.mmm.ucar.edu/wrf/users/pub-doc.html). With this assumption in place, the remainder of this chapter provides a quick overview of the methodology for downloading the WRF-Chem code, setting the required environmental variables, and compiling the WRF-Chem model. Subsequent chapters assume that the user has access to the WRF-Chem model- and emission-data sets for their region of interest and has them readily available so that a full weather and chemical transport simulation can be conducted.

2.2 Building the WRF-chemistry code

2.2.1 Getting the code

To obtain the WRF-Chem model one should follow these steps:

- Download, or copy to your working space, the WRF zipped tar file.
  - The WRF model and the chemistry code directory are available from the WRF model download web site (http://www.mmm.ucar.edu/wrf/users)
  - The chemistry code is a separate download from the WRF model download web page and can be found under the WRF-Chemistry code title
  - Always get the latest version if you are not trying to continue a long project
  - Check for known bug fixes for both WRF and WRF-Chem by examining the WRF and WRF-Chem web pages

- Unzip and untar the file
  - > gzip –cd WRFV3-Chem-3.5.TAR | tar –xf –
  - Again, if there is a newer version of the code use it, 3.5 is used only as an example
  - > cd WRFV3

Remember that bug fixes become available on a regular basis and can be downloaded from the WRF-Chem web site (http://www.wrf-model.org/WG11). You should check this web page frequently for updates on bug fixes. This includes also updates and bug fixes for the meteorological WRF code (http://www.mmm.ucar.edu/wrf/users).

2.2.2 UNIX environment settings for WRF-Chem

Before building the WRF-Chem code, several environmental settings are used to specify whether certain portions of the code need to be included in the model build. In c-shell syntax, the important environmental settings are:

```
setenv EM_CORE 1
setenv NMM_CORE 0
```

and they explicitly define which model core to build. These are the default values that are generally not required. The environmental setting

```
setenv WRF_CHEM 1
```

explicitly defines that the chemistry code is to be included in the WRF model build, and is required for WRF-Chem. This variable is required at configure time as well as compile time.

Optionally,

setenv WRF_KPP 1
setenv YACC '/usr/bin/yacc –d'
setenv FLEX_LIB_DIR /usr/local/lib

explicitly defines that the Kinetic Pre-Processor (KPP) (Damian et al. 2002; Sandu et al. 2003; Sandu and Sander 2006) is to be included in the WRF-Chem model build using the flex library (libfl.a). In our case, the flex library is located in /usr/local/lib and compiles the KPP code using the yacc (yet another compiler compiler) location in /usr/bin. This is optional as not all chemical mechanisms need the KPP libraries built during compilation. The user may first determine whether the KPP libraries will be needed (see chapter 6 for a description of available options). One should set the KPP environmental variable to zero (setenv WRF_KPP 0) if the KPP libraries are not needed.

2.2.3 Configuring the model and compiling the code

The WRF code has a fairly complicated build mechanism. It tries to determine the architecture that you are on, and then present you with options to allow you to select the preferred build method. For example, if you are on a Linux machine, the code mechanism determines whether this is a 32-or 64-bit machine, and then prompts you for the desired usage of processors (such as serial, shared memory, or distributed memory) and compilers. Start by selecting the build method:

- > ./configure

- Choose one of the options
  - Usually, option "1" is for a serial build. **For WRF-Chem do not use the shared memory OPENMP option (smpar, or dm + sm)** as these options are not supported. The serial build is a preferred choice if you are debugging the program and are working with very small data sets (e.g. if you are developing the code). Since WRF-Chem uses a lot of memory (many additional variables), the distributed memory options are preferred for all other cases

- You can now compile the code using
  - > ./compile em_real >& compile.log

- If your compilation was successful, you should find the executables in the "main" subdirectory. You should see ndown.exe, real.exe, and wrf.exe listed
  - > ls -ls main/*.exe

2.2.4 Building the WRF-chemistry-emissions-conversion code

After building the WRF-Chemistry model, you can then compile the optional conversion programs that will allow you to run the anthropogenic- and biogenic-

emissions programs. These programs are used to convert "raw" anthropogenic- and biogenic-data files into WRF netCDF input data files. In the WRFV3 directory, type the following commands:

- > ./compile emi_conv

- > ls -ls WRFV3/chem/*.exe
  - You should see the file convert_emiss.exe listed in the chemistry directory. This file should already be linked to the WRFV3/test/em_real directory.

- > ls -ls WRFV3/test/em_real/*.exe
  - You should see the files ndown.exe, real.exe, wrf.exe, convert_emiss.exe, listed in the em_real directory.

At this point all of the WRF-Chemistry model have been built. The model can be run and the run time messages should indicate that chemistry is included. But before one can use the WRF chemistry model to its full potential, the emissions input data needs to be generated. The manufacturing of the emissions input data is the subject of the next chapter.

Chapter 3: Generation of WRF-Chem-Emissions Data

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3.1 Introduction

One of the main differences between running with and without chemistry is the inclusion of additional data sets describing the sources of chemical species. At this time, these files need to be prepared externally from the WRF-Chem simulation due to the wide variety of data sources. This places the WRF-Chem user in a position of needing to understand the complexity of their emissions data as well as having the control over how the chemicals are speciated and mapped to their simulation domain. While this can be a daunting task to the uninitiated, the following section will illustrate the methodology through which emissions data is generated for a forecast domain.

3.2 Preparation of anthropogenic emissions for use with WRF-Chem

At this time there is no single tool that will construct an anthropogenic- emissions data set for **any domain and any chemical mechanism** that you select. **This places the requirement upon you, the WRF-Chem model user, to construct the anthropogenic-emissions data set for your particular domain and desired chemistry.** However,

several programs and data sets are provided that you may use to create an emissions data set, if your domain and your choice of chemical mechanism follow some restrictions. These programs are described in the following two subsections. Note that you must know *a priori* the preferred domain location and chemistry options that will be used in the simulation. The "raw" anthropogenic-emissions data set described next can be used if the domain is (1) located either anywhere over the globe, or (2) over the 48 contiguous states of the United States. The next section shows the suggested methodology for constructing your own anthropogenic-emissions data set for either one of the two domain locations.

3.2.1 Using the global-emissions data set

The use of a global-emissions data set with WRF-Chem is probably the most common choice of options. The global emissions data comes from the REanalysis of the TROpospheric (RETRO) chemical composition over the past 40 years (http://retro.enes.org/index.shtml) and Emission Database for Global Atmospheric Research (EDGAR) (http://www.mnp.nl/edgar/introduction). Both RETRO and EDGAR provide global annual emissions for several greenhouse gases (e.g., CO_2, CH_4 and N_2O) as well as some precursor gases on a .5x.5 degree (RETRO) or a 1x1 degree (EDGAR) grid.

A simple grid-mapping program has been made available to WRF-Chem users. This program, called prep_chem_sources, was developed at CPTEC, Brazil and is available to WRF-Chem users (Freitas et al., 2011). The program will map the global anthropogenic emissions data to a WRF-forecast domain using a Mercator, polar stereographic or Lambert conformal projection. This global anthropogenic emissions program and associated RETRO/EDGAR emissions is available from the WRF-Chem ftp site (ftp://aftp.fsl.noaa.gov/divisions/taq/global_emissions). The reader is advised to turn to appendix (B) for more information regarding the location of the prep_chem_sources code and global emissions data as well as the compilation and use of the prep_chem_sources routine.

3.2.2 The standard 4-km resolution data set (2005 NEI emissions data for USA only)

Anthropogenic-emissions data is currently available for the contiguous 48 states of the United States, southern Canada and northern Mexico based upon the U.S. Environmental Protection Agency (EPA) National Emissions Inventory (NEI) 2005 inventory. Area type emissions are available on a structured 4-km grid, while point type emissions are available by latitude and longitude locations and with stack parameters needed for plume-rise calculations. This data is discussed later in this section and can be found online at http://ruc.noaa.gov/wrf/WG11/anthropogenic.htm. For those who desire to conduct simulations over other regions of the world, the reader is referred to the previous section as well as appendix B that describes the use of a global anthropogenic-emissions inventory for the WRF-Chem model. The methodology for transferring an anthropogenic-emissions data set to the WRF model is discussed in the following section.

3.2.2.1 Anthropogenic-emissions construction methodology for WRF-Chem

The methodology for constructing your own anthropogenic-emissions data set is:

- Obtain the "raw" anthropogenic-emissions data. This data could come from a variety of data sources and be on multiple map projections and/or domains.
  - A 4-km emissions data set (area) and point source is available for the U.S. (ftp://aftp.fsl.noaa.gov/divisions/taq/emissions_data_2005). Use of this data is recommended when the simulation domain has a horizontal grid spacing of 12 km or greater.
- Specify, or make a table listing that relates "raw" emissions to the speciation of the desired chemical mechanism and PM mechanism (see following section)
  - The provided routines (emiss_v03.F) assume that the RADM2 chemical mechanism and MADE/SORGAM modal aerosol models are being used in the simulation.
- Prepare the 3-D (or 2-D) anthropogenic-emissions data set
  - Account for rise of emissions from stack, biomass burning, etc.
  - Output data in an intermediate format (binary for the U.S. NEI05 case). You can change format to match your needs in module_input_ chem_data.F
- Convert the emissions data to a WRF netCDF data file
  - Convert intermediate format (binary) emissions to 4-D WRF netcdf files (with executable of convert_emiss.F subroutine)
  - Input data format must match that used in the conversion routine (see module_input_chem_data.F)
  - Map data (extracted from the header in file wrfinput_d01) is needed for some plotting routines to function properly.
- If running WRF-Chem with a carbon bond type mechanism (CBM4, CBMZ, etc.), be sure to use the correct emiss_inpt_opt setting for the chemical mechanism. The WRF-Chem code will assume the emissions are in RADM2 form and will repartition the emitted species to the appropriate carbon bond mechanism unless you specify a different choice with the emiss_inpt_opt. In addition, the SORGAM emissions will be converted to the 4 or 8 size bins for use in the MOSAIC aerosol routines.

3.2.2.2 Construction of an anthropogenic-emissions-inventory conversion table

Begin with a list of known chemical species that are emitted in the domain of interest. These species may need to be translated into a list of chemical species that are used by your particular photochemical and aerosol mechanisms within the WRF-Chemistry model. If you are uncertain about the names and units of the emissions data, the registry.chem file in the WRFV3/Registry subdirectory contains the names and dimensions of the chemical species used within the WRF-Chem model.

The translation from "raw" to WRF-Chem species emissions will often result in either lumping several emitted chemical species into one simulated species, or the

partitioning of one emitted species into fractions of several simulated species. As an example, the following emission assignment table (Table. 3.2) translates the "raw" NEI05 based emission species into the WRF-Chem RADM2 species. The columns contain the following information:

- names of the emitted species in the "raw" data derived from the EPA NEI05 inventory, VOC speciation is that used in the SAPRC-99 chemical mechanism.
- names of the emitted species used in the WRF-Chemistry model, Variable names (e.g. e_co) must match the WRF-Chem Registry names of the emission variables.
- the fractional amount of the "raw" emitted species assigned to the model emission name,
- the molecular weight (used as a switch in emiss_v03.F – applies only to primary NOx, SO_2, CO and NH_3 emissions),
- the technical name of the "raw" emitted species

Table 3.1. Conversion table within emiss_v03.F used to produce input-emissions data for a WRF-chemistry simulation. This table lists the "raw" emission name, the emissions field name used in the WRF model, the weight factor applied to the chemical field, the molecular weight of the species (NOx, SO_2, CO and NH_3 only) and the full species name. The fields are then converted to an emissions speciation suitable for use with the RADM2 chemical mechanism (+MADE/SORGAM aerosol module).

"raw" name	WRF/Chm name	Weight	MW	Species name
CO	e_co	1.00	28	Carbon monoxide
NOX	e_no	1.00	46	Nitrogen Oxides (NO or NO_2)
SO2	e_so2	1.00	64	Sulfur dioxide
NH3	e_nh3	1.00	17	Ammonia
HC02	e_eth	1.00	00	Alkanes with kOH<500/ppmv/min (Ethane)
HC03	e_hc3	1.00		Alkane500<kOH<2500 (exclude C3H8, C2H2, organic acids)
HC04	e_hc3	1.11	00	Alkane2500<kOH<5000 (exlude butanes)
HC05	e_hc5	0.97	00	Alkane 5000<kOH<10000 (exlude pentanes)
HC06	e_hc8	1.00	00	Alkane kOH>10000
HC07	e_ol2	1.00	00	Ethylene
HC08	e_olt	1.00	00	Alkene kOH <20000 /ppm/min
HC09	e_oli	1.00	00	Alkene kOH >20000 /ppm/min
HC10	e_iso	1.00	00	Isoprene
HC12	e_tol	1.00	00	Aromatic kOH <20000 /ppm/min (exclude benzene and toluene)
HC13	e_xyl	1.00	00	Aromatic kOH >20000 /ppm/min (exclude xylenes)
HC14	e_hcho	1.00	00	Formaldehyde
HC15	e_ald	1.00	00	Acetaldehyde
HC16	e_ald	1.00	00	Higher aldehydes
HC17	e_ald	1.00	00	Benzaldehyde
HC18	e_ket	0.33	00	Acetone

HC19	e_ket	1.61	00	Methylethyl ketone
HC20	e_ket	1.61	00	PRD2 SAPRC-99 species (ketone)
HC21	e_hc3	0.40	00	Methanol
HC22	e_ald	1.00	00	Glyoxal
HC23	e_ald	1.00	00	Methylglyoxal
HC24	e_ald	1.00	00	Biacetyl
HC25	e_csl	1.00	00	Phenols
HC26	e_csl	1.00	00	Cresols
HC27	e_ald	0.50	00	Methacrolein
HC27	e_olt	0.50	00	Methacrolein
HC28	e_ket	0.50	00	Methylvinyl ketone
HC28	e_olt	0.50	00	Methylvinyl ketone
HC29	e_ket	1.00	00	IPRD SAPRC-99 species (other ketones)
HC31	e_olt	1.00	00	Propylene
HC32	e_hc3	0.40	00	Acetylene
HC33	e_tol	0.29	00	Benzene
HC34	e_hc3	1.11	00	Butanes
HC35	e_hc5	0.97	00	Pentanes
HC36	e_tol	1.00	00	Toluene
HC37	e_xyl	1.00	00	Xylenes
HC38	e_hc3	0.57	00	Propane
HC39	e_oli	1.00	00	Dienes
HC40	e_olt	1.00	00	Styrenes
HC41	e_ora2	1.00	00	Organic Acids
PM01	e_pm25i	0.20	01	Unspeciated primary PM2.5 - nuclei mode
PM01	e_pm25j	0.80	01	Unspeciated primary PM2.5 - accumulation mode
PM02	e_so4i	0.20	01	Sulfate PM2.5 - nuclei mode
PM02	e_so4j	0.80	01	Sulfate PM2.5 - accumulation mode
PM03	e_no3i	0.20	01	Nitrate PM2.5 - nuclei mode
PM03	e_noj	0.80	01	Nitrate PM2.5 - accumulation mode
PM04	e_orgi	0.20	01	Organic PM2.5 - nuclei mode
PM04	e_orgj	0.80	01	Organic PM2.5 - accumulation mode
PM05	e_eci	0.20	01	Elemental Carbon PM2.5 - nuclei mode
PM05	e_ecj	0.80	01	Elemental Carbon PM2.5 - accumulation mode
PM10-PRI	e_pm10	1.00	01	Unspeciated Primary PM10

The next step is to construct a program that reads the “raw” anthropogenic-emissions data, converts each chemical species to those used by the WRF-Chem model following the information from your particular conversion table and finally maps it onto the 3-dimensional simulation domain. Therefore, within this step any plume rise, or above surface anthropogenic emission placement needs to be specified. Particular attention to geospatial details, such as the WRF-Chem domain grid locations, and the elevation of model vertical levels relative to the “raw ” emissions data set must be considered.

A program is provided on the WRF-Chem ftp site (ftp://aftp.fsl.noaa.gov/divisions/taq/emissions_data_2005) that can be used with the NEI-05 U.S. anthropogenic-emissions inventory - emiss_v03.F. While your application may not use the "raw" emissions data for your simulation, it is provided as an example of the adopted methodology. The product of the program is a binary data file containing three-dimensional emissions data, output at each hour that is mapped to a specified simulation domain. The data format in the provided program is provided in Table 3.2.

Table 3.2. Converted or "intermediate binary" emission data used to produce input emissions data for a WRF-chemistry simulation. This table lists each output variable, its variable declaration, dimensions, and any additional information. The output-data fields are specific to the RADM2-chemical mechanism (+MADE/SORGAM aerosol module).

File variable	Declaration	Dimensions	Comments
nv	integer	1	Number of chemical species
ename	character*9	30	Name of each emissions field in model
hour	integer	1	Hour of the emissions data (begin loop)
so2	real	(nx,nz,ny)	
no	real	(nx,nz,ny)	
ald	real	(nx,nz,ny)	
hcho	real	(nx,nz,ny)	
ora2	real	(nx,nz,ny)	
nh3	real	(nx,nz,ny)	
hc3	real	(nx,nz,ny)	
hc5	real	(nx,nz,ny)	
hc8	real	(nx,nz,ny)	
eth	real	(nx,nz,ny)	
ora2	real	(nx,nz,ny)	
nh3	real	(nx,nz,ny)	
co	real	(nx,nz,ny)	
ol2	real	(nx,nz,ny)	
olt	real	(nx,nz,ny)	
oli	real	(nx,nz,ny)	
tol	real	(nx,nz,ny)	
xyl	real	(nx,nz,ny)	
ket	real	(nx,nz,ny)	
csl	real	(nx,nz,ny)	
iso	real	(nx,nz,ny)	
pm2.5i	real	(nx,nz,ny)	
pm2.5j	real	(nx,nz,ny)	
so4i	real	(nx,nz,ny)	
so4j	real	(nx,nz,ny)	
no3i	real	(nx,nz,ny)	
no3j	real	(nx,nz,ny)	

orgi	real	(nx,nz,ny)	
orgj	real	(nx,nz,ny)	
eci	real	(nx,nz,ny)	
ecj	real	(nx,nz,ny)	
pm10	real	(nx,nz,ny)	(end loop)

For spatial partitioning, the emiss_v03.F program implicitly assumes the WRF-Chem grid has a horizontal grid spacing larger than 4 km, and simple grid dumping from the "raw" 4-km domain into the specified WRF-Chem domain is appropriate. Currently no plume rise calculations directly couple WRF dynamics to anthropogenic point emissions. The emiss_v03.F routine includes some plume rise from the Brigg's formulation due to momentum lift from direct injection, and a specified horizontal wind climatology. Emissions within nested domains are also handled within emiss_v03.F by specifying mother domain map parameters, the nested domain grid resolution, and beginning x and y locations of the nested domain within the mother domain. These variable names are listed, and described further in the following section.

We assume that the anthropogenic-emissions data is updated at an hourly interval. However, the update interval is arbitrary and can be specified by you for your individual application. In addition, if the given binary format of the output data from emiss_v03.F is not functional for your needs, the data format can be modified within the program. However, if the output data format is changed, the WRF-Chem program convert_emiss.F will also need to be modified so that the converted raw-emissions data can be read into the program correctly and converted.

The emissions units for both surface and elevated point sources are in *mole per square kilometer per hour* for gas phase species and in units of *microgram per square meter per second* (microgram m^{-2} s^{-1}) for the aerosol species. These are the units assumed within the WRF-Chem input processor for the emissions files, and the convert_emiss.F processing step that generates the netcdf emission file(s) described further below. (Conversion of gas-phase emissions into the mixing ratio increases at each grid is handled within module_emissions_anthropogenic.F. Aerosol increases due to emissions are handled in individual aerosol mechanism modules.)

It is entirely incumbent upon the user to specify location and time of emissions from the "raw" emissions for their own applications within this intermediate step of the emissions processing.

3.2.2.3 Additional details for running emiss_v03.F with the NEI-05 anthropogenic-emissions data set

The "raw" anthropogenic-emissions data for the 48 contiguous states as well as select regions of Canada and Mexico have been made available for download by the NOAA/Earth System Research Laboratory, Chemical Sciences Division. The process to create anthropogenic-emissions-input data files from this data is as follows:

- Before generation of the anthropogenic-emissions data file can begin, the real.exe program should be used to create the wrfinput_d01 and wrfbdy_d01 data files for your desired domain. There are two reasons for doing this. The first is so that you know exactly where the simulation domain is located. The second is because the emissions conversion program (convert_emiss.exe) will read the netCDF header information from the wrfinput_d01 data file and write this information into the WRF-chemical-emissions data files. If the wrfinput_d01 data file does not exist, the program will abort with an error.

- Download the raw-emissions data tar file from the anonymous ftp server (ftp://aftp.fsl.noaa.gov/divisions/taq/emissions_data_2005/em05v2_file*.tar) and extract the data into its own directory (e.g., $home/emissions_data).

- Download the emiss_v03.F program from the anonymous ftp server.

- Modify emiss_v03.F to set map and grid parameters for your particular domain as well as the directory that contains the "raw" emissions data. For the provided test domain you should have the following settings:

Model variable	Value	Description
Il	40	east-west grid spacing (ix2+1) of mother domain and west_east_stag dimension on your WRF domain
Jl	40	north-south grid spacing (jx2+1) of mother domain and south_north_stag dimension on your WRF domain
Ix2	39	x-dimension of user domain output data (IL-1)
Jx2	39	y-dimension of user domain output data (JL-1)
Kx	19	z-dimension of user domain output data or kemit on your WRF domain. The vertical dimension can equal or be less than that used in the WRF domain.
Inest1	0	nesting or no nesting flag (no nesting => inest1 = 0)
Dx	60.E3	horizontal grid spacing (m) of user domain
Dxbigdo	60.E3	Horizontal grid spacing on mother domain (m)
Xlatc	38.00	grid center latitude of mother domain
Xlonc	-80.00	grid center longitude of mother domain
Clat1	38.001	Northern most reference latitude of projection (mother domain)
Clat2	38.000	Southern most reference latitude of projection (CLAT1 > CLAT2 for Lambert Conformal, CLAT2 not used for polar stereographic)
Iproj	1	projection type (see WRFSI information)
Rekm	6370.	Earth radius (km)
XNESSTR	1.	x-location in mother domain of southwest corner point of the (1,1) grid in the user domain. Not used if Inest1=0 .
YNESSTR	1.	y-location in mother domain of southwest corner point of the (1,1) grid in the user domain. Not used if Inest1=0 .
Datadir	/data	Path to directory holding emissions input data (character string)
Zfa	(See below)	Elevation (m) at the top of each computational cell
KWIN	20	Number of vertical levels in the horizontal wind profile
WSP		Wind speed at level height(m) specified by REFWZ
REFWZ		Elevation (m) of the specified horizontal wind profile

```
DATA ZFA/  0.,  255.,  515.,  781., 1054., 1335.,  &
        1527., 1824., 2130., 2553., 2994., 3454.,  &
        4059., 4967., 6741., 8723.,10992.,14084.,  &
       16461.,20346./
```

Note: the model ZFA height levels have been determined separately by processing the wrfinput_d01 file generated by real.exe to obtain the average height of each vertical domain levels in meters.

- Compile emiss_v03.F (single processor mode) with the command "pgf90 –Mfree –byteswapio –o emiss_v03.exe emiss_v03.F" and run emiss_v03exe. This program, using raw-emissions data, maps the emissions data to your specified domain and generates binary-emissions data files (file names are set in emiss_v03.F to be wrfem_00to12Z and wrfem_12to24Z).

3.2.3 Wildfire emissions

The prep_chem_sources program (see appendix B) is capable of providing biomass burning emissions or wildfire emissions to the WRF-Chem forecast. The geostationary NOAA weather satellite (GOES) provides half-hourly fire data for the Western Hemisphere. Specifically, GOES-East provides coverage for North and South America while GOES-West covers North America only. Data files containing the WFABBA fire location are distributed by the University of Wisconsin-Madison (http://cimss.ssec.wisc.edu/goes/burn/wfabba.html). The archived WF-ABBA data are available at this time from two different web sites; http://www.firedetect.noaa.gov and http://www.nrlmry.navy.mil.flambe/index.html. Additional wildfire location data is available from MODIS at the University of Maryland web site: http://firefly.geog.umd.edu/firms. The prep_chem_sources reads this data, the WFABBA data files all being in one directory and MODIS from the same or different directory, and maps the point source data to the WRF domain. It is also not too difficult to include other sources for wildfire emissions.

In the WRF-Chem model, the wildfire-emissions data is obtained from the wrffirechemi_d01 emissions data file. It computes the plume rise of the wildfire smoke based upon the environmental wind and temperature profile. The emissions to the forecast are then provided as a vertical distribution based upon the results from the plume rise calculation.

3.2.4 Volcanic emissions

In this section the ash and SO_2 emissions from prescribed volcanic activities is described. For additional information on volcanic emissions that are produced when running prep_chem_sources the reader is referred to Freitas et al., 2011.

3.2.4.1 Volcanic ash emissions

To determine ash emission field during volcanic eruption events, prep_chem_sources follows the database developed by Mastin et al. (2009). This database provides a set of parameters to model volcanic ash cloud transport and dispersion during eruptions. There is information on 1535 volcanoes around the world comprising location (latitude, longitude and height) and the corresponding parameters plume height, mass eruption rate, volume rate, duration of eruption and the mass fraction of erupted debris finer than about 63 μm are provided. The emissions preprocessing tool provides the place of the volcano in the nearest model grid box and the corresponding emission parameters (mass eruption rate, plume height and duration). Then this information is used within WRF-Chem to determine the vertical distribution of the erupted mass. Within the modeling transport system, 75% of the erupted mass is detrained in the umbrella cloud and 25% beneath. The base of the umbrella cloud is roughly located at 73% of the plume height. The total erupted mass is calculated using the correspondent erupted volume times the ash mass density, which is defined as being 2,500 kg m^{-3}.

The total ash mass is distributed between 10 bins of aerosol particles with diameter size range starting from 2 mm down to less than 3.9 μm, using the correspondent percentage of mass described by the Mount Saint Helens eruption of 1980 (Carey and Sigurdsson, 1982). For each bin, the aerodynamic radius, needed by the setting velocity calculation, is defined as half of the arithmetic mean between the limits of the diameters of each bin size. The algorithm to calculate the settling velocity was originally developed for the GOCART model (Chin et al., 2002). This calculation is based on the Stokes law corrected by the Cunningham slip factor (Pruppacher and Klett, 1997). The time interval which the ash mass is released in the domain of the model simulation is given by the 'duration' parameter specified in the volc_emissions.f90.

3.2.4.2 Volcanic SO_2 degassing emissions

The data provided by the AEROCOM program (http://www-lscedods.cea.fr/aerocom/AEROCOM_HC/volc/, Diehl, 2009, Diehl et al., 2011) contains volcanic SO_2 emissions and other variables for all days from 1 January 1979 to 31 December 2007 for all volcanoes with historic eruptions listed in the Global Volcanism Program database provided by the Smithsonian Institution. There is one file for each year that contains the number of events for each day of that year over the entire world. For each event, the volcano name, date, height above the mean sea level, cloud column height, longitude, latitude and daily emission rate of SO_2 are provided. There is also a separation between eruptive and non-eruptive volcanic emissions.

In similar fashion to the volcanic ash, the emissions processing code prep_chem_sources places the SO_2 emissions from each volcano in the grid box which surrounds its geographical location. The total emission is calculated by summing the emissions of all volcanoes within the grid cell. Next, the total emission and the minimum and maximum column heights of the set of volcanoes within the grid cell are provided. The units are kg [SO_2] m^{-2} dy^{-1}.

3.3 Generating the netcdf-emissions data sets

The final step in the process is to produce a WRF-Chem netCDF-emissions input data file containing all of the required metadata (map projection data, simulation start time, etc.) for the simulation. Ideally the metadata contained in the WRF-Chem-emissions file would be generated by the previous step. However, if not provided by the user, the WRF input data file (e.g., wrfinput_d01) can be read and the metdata information added to the anthropogenic-emissions input data file. The name of the final netcdf data file(s) can be either wrfchemi_<hour>_d<domain_id> or wrfchemi_d<domain_id>_<date/time> depending upon your intent (io_style_emissions option in namelist). The latter intent is designed for daily varying emissions (io_style_emissions=2), and in this case the date/time specified in the WRF-Chem-emissions data file must match the simulation date/time or no emissions data will be read and a run-time error will result. The first intent (io_style_emissions=1) assumes you are creating two netcdf 4-D emission files named wrfchemi_00z_d<domain_id> and wrfchemi_12z_ d<domain_id> that contain hourly emissions from 00:00 to 11:00 UTC, and 12:00 to 23:00 UTC, respectively. This is the format generated by convert_emiss.F that matches the provided NEI-05 inventory. The NEI-05 inventory is representative of a "typical ozone season day" by the U.S. EPA, and is typically used for all days within multiday WRF-Chem simulations.

- Before the conversion from "binary intermediate" to netcdf file emissions can begin, you need to change the namelist.input file in the WRFV3/test/em_real directory to the emissions data file settings. The settings that will generate 24 hours of hourly-emissions (i.e., io_style_emissions=2) data are:

```
&time_control
run_days                = 1,
run_hours               = 0,
run_minutes             = 0,
run_seconds             = 0,
start_year              = 2008,
start_month             = 07,
start_day               = 14,
start_hour              = 00,
start_minute            = 00,
start_second            = 00,
end_year                = 2008,
end_month               = 07,
end_day                 = 15,
end_hour                = 12,
end_minute              = 00,
end_second              = 00,
auxinput6_inname        = 'wrfbiochemi_d<domain>',
auxinput7_inname        = 'wrffirechemi_d<domain>',
auxinput8_inname        = 'wrfchemi_gocart_bg_d<domain>',
auxinput12_inname       = 'wrf_chem_input',
```

```
 auxinput13_inname          = 'wrfchemv_d<domain>',
 auxinput5_interval_m       = 60,
 auxinput7_interval_m       = 1440,
 auxinput8_interval_m       = 1440,
 io_form_auxinput2          = 2,
 io_form_auxinput5          = 2,
 io_form_auxinput6          = 2,
 io_form_auxinput7          = 2,
 io_form_auxinput8          = 2,
 io_form_auxinput12         = 0,
 io_form_auxinput13         = 2,
io_form_auxinput14          = 0,
io_form_auxinput15          = 0,
/

&chem
 chem_opt                   = 1,
 emiss_opt                  = 3,
 chem_in_opt                = 0,
 bio_emiss_opt              = 1.
```

Since version 3.3, the name list setting for the auxiliary input port time interval is now dependent upon each input stream. That is, for the emissions conversion program convert_emiss.exe, the settings for each auxiliary input port specifies whether it is turned on, the IO format, the time interval for the emissions data updates and the number of frames in each file (not shown).

- It is assumed that you have already configured and compiled the WRF-Chem model. So now build the emissions conversion program with the command "compile emi_conv" in WRFV3 directory.

- Run convert_emiss.exe for 24 hours starting at 0000 UTC and ending at 0000 UTC and save the netCDF wrfchemi_d01 data file as wrfchemi_d01_2008-07-14_00:00:00. The filename(s) need to match the name of the input data file in mediation_integrate.F (see convert_emiss.F program inside the WRFV3/chem directory). The file(s) should be transferred (or linked) to your WRFV3/test/em_real directory.

- Once the "wrfchemi" files are generated, it is best to plot fields or use a program like ncview to examine the files that have been generated. Look at the files and confirm that the emissions appear to match the WRF forecast domain you previously generated. When looking at anthropogenic emissions (e.g., co) the surface emissions should look similar to a map with cities and possibly roads showing. Be sure to confirm that the fields are consistent with your expected emissions fields in both space (vertically) as well as in time. If the emissions do not match, then a dimension error is likely happened in your namelist.input file.

3.4 Construction and preparation of tracer emissions

At this time there is no single program available that will allow the user to construct tracer emissions for their domain and directly import them into the simulation. However, there are relatively simple methodologies that can be undertaken to allow the user to generate their tracer emissions.

Probably the simplest way to produce tracer emissions is to modify the program emiss_v03.F to suit your needs. Upon examination of the emiss_v03.F program one will see that it can be modified to skip the reading of the NEI emissions data sets and instead fill the output array. The output array (i.e., EM3RD(I,K,J,N)) can be filled with user-specified values at the desired grid location with the user-specified emitted tracer amount. The user needs to be aware of not only where the emitted species are to be located in their simulation domain (grid indexes I,K and J)), but also which chemical emissions index, N, corresponds to the emitted species used as a tracer in their simulation. To get the emissions correct, start by examining the registry.chem file to determine which species are used in the tracer package (chem._opt=13). Then use the array ENAME in the emiss_v03.F program to get the name and order of the emitted species. Then one can set the emissions for the correct chemical index in the output array. Once the modified program has been compiled and run, the binary intermediate file containing the emitted tracer data will need to be converted to a WRF netCDF input file using the convert_emiss.F program discussed in the previous section. An example routine using this methodology has been made available on the WRF-Chem ftp server at: ftp://aftp.fsl.noaa.gov/divisions/taq/emissions_data_2005/emiss_v03_tracer.F

Another methodology is for the user to build their own tracer-emissions data file and use the convert_emiss.F program as is, or modified as needed, to read the tracer data file and produce a tracer emissions input file. This option allows users to use pre-existing data files and to modify the tools available with the chemistry to produce input or output files for their needs depending upon the emissions options selected.

3.4.1 The CO_2 tracer option

The CO_2 tracer option allows a user to simulate biospheric CO_2 fluxes using Vegetation Photosynthesis and Respiration Model coupled to WRF-Chem. The VPRM model uses satellite data and WRF meteorology to derive biospheric CO_2 fluxes from different biomes. All the chemistry species such as CO_2 and CO in this option are treated as passive tracers. No chemistry and removal processes are considered for this option. The option simulates transport and mixing of several CO_2 and CO tracers from different sources such as background, anthropogenic and biospheric. More information regarding VPRM is provided by Pillai et al., 2011 and Ahmadov et al., 2009.

3.4.2 The Greenhouse Gas tracer option

The Greenhouse Gas tracer option allows a user to perform simulations of CO_2, CO, and CH_4 within WRF-Chem. All chemistry species are treated as passive tracers. The option includes all tracers from the CO_2 tracer option but also includes CH_4 tracers (biogenic, anthropogenic, background) and biomass burning tracers for CO_2, CO, and CH_4 as well. Biogenic CH_4 fluxes are simulated with the Kaplan wetland inventory, the soil uptake model from Ridgwell, and the termite database of Sanderson coupled to WRF-CHEM. The flux models use WRF meteorology and soil characteristics to calculate the CH_4 fluxes. The wetland inventory additionally relies on an external wetland inundation map and carbon pool. Similar to chem_opt=16 no chemistry and removal processes are considered. Detailed information is found in Beck et al. (2011).

3.5 Preparation of biogenic emissions

The WRF-chemistry model does have four options to compute the biogenic-emissions data. These options are:

3.5.1 No biogenic emissions

The first option is not to use an additional biogenic-emissions input data file (bio_emi_opt= 0). The user could add the biogenic-emission to the anthropogenic-emissions data if it is desired. Be sure to do this for every time period in the emissions input data and not just the first time.

3.5.2 Guenther biogenic emissions

For the second option (bio_emi_opt= 1), the model calculates the biogenic emissions online using the USGS land-use classification, which is generated by WRF WPS and available for the meteorological and chemical model. The user does not prepare any biogenic-emissions input data set.

3.5.3 BEIS 3.14 biogenic emissions

For the third option, the user specifies reference fields for the biogenic emissions, which are then modified online by a subroutine from the Biogenic-Emissions Inventory System (BEIS) version 3.14. The land use for this emissions inventory is obtained from the Biogenic-Emissions Land-use Database version 3 (BELD3). The reference fields need to be provided as an additional input data file (wrfbiochemi_d01) for the real.exe program.

The BEIS3.14 model is publicly available through the CMAS (Community Modeling and Analysis System) at http://www.cmascenter.org/ as part of the SMOKE (Sparce Matrix Operator Kernel Emissions) software package (version 2-4). The physical parameterizations for temperature, light dependencies, and canopy light correction are contained within module_bioemi_beis314.F of WRF-Chem. Reference emission files (30°C, 1000 PAR) from BEIS3.14 rely on the BELD3 (Biogenic Emissions Landuse Database, version 3) available at

http://www.epa.gov/ttn/chief/emch/biogenic/. This North American database contains fractional area information on 230 individual forest, grass, and crop types at 1-km horizontal resolution. Tools for spatial allocation of BELD3 data into common user defined grids are also available at that website. As part of the reference emission pre-processing, BEIS3.14 contains season-specific and vegetation-specific information for emissions of 33 individual VOC species (including isoprene and 14 monoterpenes), biogenic/agricultural NO, and LAI (Leaf Area Index) information needed in the canopy light dependence calculations of isoprene, methanol and methyl-butenol.

The current version of module_bioemi_beis314.F is specific to reference emissions generated for the RADM2 or RACM chemical mechanism by NOAA/ESRL/CSD. Reference emissions for 15 VOC species within RACM, 3 NO emission classes, and the LAI field specific to isoprene are each output on a 2-dimensional grid for the defined WRF-Chem simulation grid as simple ASCII files having the dimensions of (nx-1,ny-1), in 12E9.2 format. This input format is defined, and modifiable within the input_ext_chem_beis3_file routine in WRFV3/chem/module_input_chem_bioemiss.F. Units of emissions are in mole/km^2/hr within the ASCII files, the same as other gas-phase emissions. A list of biogenic emission variables specific to the RACM species assignment is given in table 3.3.

Table 3.3. List of biogenic-emission variable names, and their RACM mechanism meaning.

File variable	Comments
Iso	Isoprene
Oli	Internal Olefins
Api	Alpha Pinene
Lim	Limonene
Xyl	Xylene
hc3	Alkane500<kOH<2500 (propane)
Ete	Ethylene
Olt	Terminal Olefins
Ket	Ketones
Ald	Acetaldehyde (and higher aldehydes)
Hcho	Formaldehyde
Eth	Ethane
ora2	Acetic and higher organic acids
Co	Carbon Monoxide
Nr	Nonreactive VOC
noag_grow	Agricultural NO – fertilized growing
noag_nongrow	Agricultural NO – nonfertilized growing
Nononag	Nonagricultural NO
Slai	LAI for isoprene emissions

The program convert_emiss.F must be compiled, and the executable convert_emiss.exe must be run. A data file called wrfbiochemi_d01 (for domain 1) will be created if bio_emiss_opt = 2 in your namelist.input file. Run real.exe (with bio_emi_opt=2 in the namelist) when creating the wrfinput data file - the biogenic emissions variables should now be included in the wrfinput data file.

3.5.4 MEGAN biogenic emissions

The final option for biogenic emissions is the use of the Model of Emissions of Gases and Aerosols from Nature (MEGAN). This global biogenic-emissions data set has a horizontal spatial resolution of approximately 1 km so it can be used for nearly any WRF-Chem simulation. The use of this biogenic-emissions option requires the user to download and compile a further utility from the National Center for Atmospheric Research (NCAR) web site http://www.acd.ucar.edu/wrf-chem/. The utility prepares MEGAN input data files for use in WRF-Chem – these files are named wrfbiochemi_d0x files – and a separate file is provided for each domain (d0x). The assimilation of MEGAN biogenic emissions into WRF-Chem is a matter of setting the correct namelist.input settings. Further instructions, including support contact details at NCAR, can be found in Appendix C.

3.6 Conversion of biogenic-emission data files

The emissions-input data files for biogenic and biomass-burning data also need to be in a WRF input data file format. This includes containing the correct header information related to your simulation domain. There is a program available that converts the emissions data from their respective intermediate data files to a WRF chemical-emissions input file – convert_emiss.exe. This program is located under the WRFV3/chem directory and is compiled using the compile emi_conv command. The executable can be located in the WRFV3/test/em_real directory. The program will read the namelist.input file and convert the data files depending upon the options set by the user in the chemistry and time_control namelists.

3.7 Placement of chemical-emission input data files

The emissions-input data files need to be located either in the run or the test/em_real directory. Often users place the data in the run directory and link it the test/em_real directory, since they will be used over and over again.

As you can see from this example, the WRF-Chem anthropogenic-emissions data file (wrfchemi_d01_2008-07-14_12:00:00) is located in the WRFV3/run directory and is linked to the WRFV3/test/em_real directory. One advantage of this methodology is the reduced chance of accidentally removing the data files. It also reduces disk space usage as only one data file is needed, and it could allow for one data file to be used for multiple simulations by changing the name of the linked data file.

Chapter 4: Running the WRF-Chemistry Model

Table of Contents

4.1 Introduction

After successful construction of the anthropogenic- and biogenic-emission-input data files, it is time to run the model. This process is no different than running the meteorological version of the model. To make an air-quality simulation, change directory to the WRFV3/test/em_real directory. In this directory you should find links to the executables real.exe, and wrf.exe, other linked files, and one or more namelist.input files in the directory.

For larger domain simulations, one should use a DM (distributed memory) parallel system to make a forecast. This is of particular importance for WRF-Chem since much additional memory is required.

4.2 WRF-Chem name list options: the choice of CHEM_OPT

The largest portion of the chemistry name list options are related to the chemical mechanisms and aerosol modules selection. The mechanism used during the forecast is decided with the name list parameter chem_opt that is described next. Some of these choices require other settings for other name list options. The options that are printed with red lettering indicate those options that are not fully implemented and tested. Model users are discouraged from selecting those options as they are not fully supported and could produce erroneous, or in the extreme case, detrimental results. In addition, it should be pointed out that the model developers most often work with just a few options at one time (e.g., RADM2/MADE-SORGAM, CBMZ/MOSAIC). Not all of the other available options are tested during development, but often it is a trivial exercise to make the other options functional. Therefore, users are encouraged to determine their desired settings that works best for their simulation, test the name list combination, improve the model

code, and then communicate the improvements to the WRF-Chem user community. The chem_opt name list parameter is organized according to the chemical mechanism that is used.

	&chem namelist variable	Description	Additional Comments
	chem_opt = 0	no chemistry	
RADM2 /QSSA Chemistry	= 1	includes chemistry using the RADM2 chemical mechanism - no aerosols	
	= 2	includes chemistry using the RADM2 chemical mechanism and MADE/SORGAM aerosols.	
	= 5	CBMZ chemical mechanism with Dimethylsulfide, or DMS	
	= 6	CBMZ chemical mechanism without DMS	
	= 7	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 4 sectional aerosol bins.	
	= 8	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 8 sectional aerosol bins.	
	= 9	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 4 sectional aerosol bins including some aqueous reactions	For dust and sea salt use dust_opt=2, seas_opt=2
	= 10	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 8 sectional aerosol bins including some aqueous reactions	For dust and sea salt use dust_opt=2, seas_opt=2.
	= 11	RADM2 chemical mechanism and MADE/SORGAM aerosols including some aqueous reactions	For dust and sea salt use dust_opt=2, seas_opt=2.
	= 12	RACM chemical mechanism and MADE/SORGAM aerosols including some aqueous reactions	For dust and sea salt use dust_opt=2, seas_opt=2.
	= 13	Run with 5 tracers with emissions, currently set up for SO_2, CO, no, ald, hcho, ora2	
	= 14	Single tracer run using tracer_1 array	Use of tracer_opt suggested
	= 15	Ensemble tracer option using 20 individual tracers and an ensemble tracer array	Use of tracer_opt suggested
	= 16	Greenhouse Gas CO_2 only tracer	Use of tracer_opt suggested

= 17	Greenhouse Gas tracer	
= 30	CBMZ chemical mechanism (chem_opt=6) and MADE/SORGAM modal aerosol	
= 31	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 4 sectional aerosol bin with dms	
= 32	CBMZ chemical mechanism with (chem_opt=6) and MOSAIC using 4 sectional aerosol bins with dms. Some aqueous reactions included	
= 33	CBMZ chemical mechanism (chem_opt=6) and MOSAIC using 8 sectional aerosol bin with dms. Some aqueous reactions included	
= 34	CBMZ chemical mechanism with (chem_opt=6) and MOSAIC using 8 sectional aerosol bins with dms. Some aqueous reactions included.	
= 35	CBMZ chemical mechanism (chem_opt=6) and MADE/SORGAM modal aerosol. Some aqueous reactions included	
= 41	RADM2/SORGAM with aqueous reactions included.	
= 42	RACM/SORGAM with aqueous reactions included (KPP)	Includes less complex aqueous reactions following CMAQ methodology, SO4 and NO3 wet deposition
= 43	NOAA/ESRL RACM Chemistry and MADE/VBS aerosols using KPP library. The volatility basis set (VBS) is used for Secondary Organic Aerosols	Includes less complex aqueous reactions following CMAQ methodology, SO4 and NO3 wet deposition
= 101	RADM2 Chemistry using KPP library	Includes less complex aqueous reactions following CMAQ methodology
= 102	RACM-MIM Chemistry using KPP library	Rosenbrock solver, can use larger time step
= 103	RACM Chemistry using KPP library	Rosenbrock solver, can use larger time step
= 104	RACM Chemistry and PM advection using KPP library	Rosenbrock solver, can use larger time step
= 105	RACM Chemistry and MADE/SORGAM aerosols using KPP library	PM total mass. This was originally implemented for wildfires
= 106	RADM2 Chemistry and MADE/SORGAM aerosols using KPP	Rosenbrock solver, can use larger time step

	library	
= 107	RACM Chemistry and MADE/SORGAM aerosols using KPP library using the ESRL chemical reaction table	Rosenbrock solver, can use larger time step
= 108	NOAA/ESRL RACM Chemistry and MADE/VBS aerosols using KPP library. The volatility basis set (VBS) is used for Secondary Organic Aerosols	Rosenbrock solver, can use larger time step
= 110	CB4 Chemistry using KPP library	Rosenbrock solver, can use larger time step
= 111	MOZART Chemistry using KPP library	Rosenbrock solver, can use larger time step
= 112	MOZART Chemistry and GOCART aerosols (MOZCART) using KPP library	Rosenbrock solver, can use larger time step. Use phot_opt=3
= 120	CBMZ Chemistry using KPP library	Rosenbrock solver, can use larger time step. Use phot_opt=3
= 170	CBMZ Chemistry with MOSAIC aerosols using KPP library	Rosenbrock solver, can use larger time step
= 195	SAPRC99 Chemistry using KPP library	Rosenbrock solver, can use larger time step
= 198	SAPRC99 Chemistry with MOSAIC using KPP library. The MOSAIC aerosols uses 4 sectional aerosol bins and includes volatility basis set (VBS) for organic aerosol evolution	Rosenbrock solver, can use larger time step
= 199	MOZART Chemistry with MOSAIC using KPP library. The MOSAIC aerosols uses 4 sectional aerosol bins and includes volatility basis set (VBS) for organic aerosol evolution	Rosenbrock solver, can use larger time step
= 200	NMHC9 Chemistry using KPP library	Rosenbrock solver, can use larger time step
= 300	GOCART simple aerosol scheme, no ozone chemistry	Only 18 variables, currently no direct or indirect effect supported Optionally use dmsemis_opt=1, dust_opt=1, seas_opt=1
= 301	GOCART coupled with RACM-KPP	Only 18 variables Optionally use dmsemis_opt=1, dust_opt=1, seas_opt=1
= 302	RADM2 Chemistry and GOCART aerosols using KPP library	Simple aerosol treatment, no indirect effect supported yet. Optionally use dmsemis_opt=1 dust_opt=1, seas_opt=1
= 303	RADM2 Chemistry and GOCART	Simple aerosol treatment. Optionally

	aerosols	use dmsemis_opt=1, dust_opt=1 seas_opt=1
= 400	Volcanic ash fall and concentration only	Simple aerosol treatment. Optionally use dmsemis_opt=1 dust_opt=1, seas_opt=1
= 401	Dust concentration only	Simple ash treatment with 10 ash size bins
= 402	Volcanic ash fall and SO_2 concentration	Simple dust treatment with 5 size bins
= 501	CBMZ with CAM-MAM3	Simple ash treatment with 10 ash size bins and volcanic SO_2 gas emissions
= 502	CBMZ with CAM-MAM7	MAM chemistry with 3 mode aerosol species. Requires CAM5 Morrison and Gettleman scheme (mp_phys=11).
= 503	CBMZ with CAM-MAM3_AQ	MAM chemistry with 7 mode aerosol species. Requires CAM5 Morrison and Gettleman scheme (mp_phys=11).
= 504	CBMZ with CAM-MAM7_AQ	MAM chemistry with 3 mode aerosol species and aqueous chemistry. Requires CAM5 Morrison and Gettleman scheme (mp_phys=11). MAM chemistry with 7 mode aerosol species and aqueous chemistry. Requires CAM5 Morrison and Gettleman scheme (mp_phys=11).

4.3 Other chemistry name list options

input_chem_inname <string>		name of chemistry input file
chem_in_opt	= 0	uses idealized profile to initialize chemistry
	=1	uses previous simulation data to initialize chemistry. The input file name will have the structure wrf_chem_input_d<domain> and the data will be read in through auxiliary input port 12
io_style_emissions	= 0	no emissions data read
	= 1	two 12-h emissions data files used
	= 2	date/time specific emissions data files used
chemdt	= 1.5	time step used by chemistry in minutes
bioemdt	= 30	update time interval used by biogenic emissions in minutes
kemit	= 8	number of vertical levels in the emissions input data file. (considering the domains namelist; 0 < kemit < e_vert)
kemit_aircraft	= 1	number of vertical levels for aircraft emissions. The aircraft emissions are read in through auxiliary input port 14
photdt	= 30	update time interval used by photolysis routine in minutes
phot_opt	= 0	no photolysis
	= 1	uses Madronich photolysis (TUV)
	= 2	uses Fast-J photolysis

	= 3	uses Madronich F-TUV photolysis (aerosol interaction is not hooked up with MOSAIC aerosols)
emiss_opt	= 0	no anthropogenic emissions
	= 2	uses radm2 anthropogenic emissions
	= 3	uses radm2/MADE/SORGAM anthropogenic emissions
	= 4	uses CBMZ/MOSAIC anthropogenic emissions
	= 5	GOCART RACM_KPP emissions
	= 6	GOCART simple emissions
	= 7	MOZART emissions
	= 8	MOZCART (MOZART + GOCART aerosols) emissions
	= 9	Converts default RADM2 gas emissions to CBMZ. Aerosol emissions are speciated to MAM 3-mode aerosols
	= 10	MOZART (MOZART + aerosols) emissions
	= 13	SAPRC99 emissions
	= 16	Greenhouse Gas CO_2 tracer emissions
	= 17	Greenhouse Gas tracer emissions
emiss_opt_vol	= 0	no volcanic ash emissions
	= 1	Include volcanic ash emissions for 10 size bins
	= 2	Include SO_2 as well as the volcanic ash emissions for 10 size bins
aircraft_emiss_opt	= 0	no aircraft emissions
	= 1	uses aircraft emissions
gas_drydep_opt	= 0	no dry deposition of gas species
	= 1	includes dry deposition of gas species
aer_drydep_opt	= 0	no dry deposition of aerosols
	= 1	includes dry deposition of aerosols
depo_fact	= 0.25	when using VBS for aerosols, the ratio between dry deposition velocities of organic condensable vapors and dry deposition of HNO_3 (default value = 0.25)
bio_emiss_opt	= 0	no biogenic emissions
	= 1	calculates biogenic emissions online using the Gunther scheme
	= 2	includes biogenic emissions reference fields in wrfinput data file and modify values online based upon the weather
	= 3	includes MEGAN biogenic emissions online based upon the weather, land use data. Need to include ne_area setting, the total number of chemical species, in the chemical namelist.
	= 16	Include CO_2 biomass emissions from the VPRM model. (Requires user to provide external files through auxiliary input port 15.)
	= 17	Include VPRM input fields, Kaplan wetland inventory input fields when chem_opt=17. (Requires user to provide external files through auxiliary input port 15.)
ne_area	= 41	Used by MEGAN biogenic emissions to provide a minimum total number of chemical species used by specified chemistry option. Best to set to a value larger than all chemical species (i.e., ne_area > 100).
emiss_inpt_opt	= 0	no emissions data read
	= 1	emissions are speciation for RADM2/SORGAM. Recommended

		when using the NEI-05 or EDGAR/RETRO emissions speciated for RADM2 chemical mechanism
	= 3	emissions are speciation for GOCART_SIMPLE from NEI-05. This is a kludge and its use is not recommended
	= 16	Used with chem_opt=16, or 17 only to add fluxes and emissions to passive tracers.
	= 101	RADM2 emission speciation adapted after reading the data file to follow the CBMZ/MOSAIC framework
	= 101	RADM2 emission speciation adapted after reading the data file to follow the CBMZ/MOSAIC framework
	= 102	RADM2 emission speciation adapted after reading data file to follow the RADM2/SORGAM framework (similar to 101, but with isoprene included)
	= 103	Carbon Bond 4-emission speciation adapted after reading the RADM2 data file
	= 104	Carbon Bond 4-emission speciation adapted after reading the RADM2 data file. Secondary Organic Aerosol (SOA) precursors computed from input data as well. Use for CAM5 micrphysics and MAM 3-mode aerosol
	= 111	RADM2 emission speciation adapted after reading data file to follow the MOZART framework
biomass_burn_opt	= 0	no biomass burning emissions
	= 1	include biomass burning emissions and plume rise calculation
	= 2	include biomass burning emissions and plume rise calculation for MOCART
	= 3	include biomass burning emissions and plume rise calculation for MOZART
	= 5	include biomass burning emissions and plume rise calculation for GHG tracers fo CO_2, CO and CH_4 (needs chem_opt=17)
plumerisefire_frq	= 180	time interval for calling the biomass burning plume rise subroutine
dust_opt	= 0	no GOCART dust emissions included
	= 1	include GOCART dust emissions - need to provide fractional erosion map data
	=2,	MOSAIC and MADE/SORGAM dust emissions option (does not requires extra input data)
	=3,	Include GOCART dust emissions with AFWA modifications
seas_opt	= 0	no GOCART sea salt emissions
	= 1	include GOCART sea salt emissions
	= 2	MOSAIC or MADE/SORGAM sea salt emissions
dmsemis_opt	= 0	no GOCART dms emissions from sea surface
	= 1	include GOCART dms emissions from sea surface - need to provide dms reference field (currently only working for GOCART options)
aer_op_opt	= 1	aerosol optical properties calculated based upon volume approximation
	= 2	aerosol optical properties calculated based upon Maxwell

		approximation
	= 3	aerosol optical properties calculated based upon exact volume approximation
	= 4	aerosol optical properties calculated based upon exact Maxwell approximation
	= 5	aerosol optical properties calculated based upon exact shell approximation
opt_pars_out	= 0	no optical properties output
	= 1	include optical properties in output
gas_bc_opt	= 1	uses default boundary profile
	= 16	sets values of CO_2, CO and CH_4 mixing ratios at boundaries to relevant constants. If a user wants to use boundary conditions from a global model, then the wrfbdy file should be modified and "have_bcs_chem" must be set to ".true."
	= 101	uses modified default boundary profile – originally designed for use at Houston, TX
gas_ic_opt	= 1	uses default initial condition profile
	= 101	uses modified default initial condition profile – designed for use at Houston, TX
	= 16	sets initial values of CO_2, CO and CH_4 mixing ratios to relevant constants
	= 101	uses modified default initial condition profile – designed for use at Houston, TX
aer_bc_opt	= 1	uses default boundary profile
	= 101	uses modified default boundary profile – designed for use at Houston, TX
aer_ic_opt	= 1	uses default initial condition profile
	= 101	uses modified default initial condition profile – designed for use at Houston, TX
gaschem_onoff	= 0	gas phase chemistry turned off in the simulation (useful for debugging)
	= 1	gas phase chemistry turned on in the simulation (default)
aerchem_onoff	= 0	aerosol chemistry turned off in the simulation (useful for debugging)
	= 1	aerosol chemistry turned on in the simulation (default)
wetscav_onoff	= 0	wet scavenging turned off in the simulation, also see the "chem_opt" parameter
	= 1	wet scavenging turned on in the simulation, also see the "chem_opt" parameter
cldchem_onoff	= 0	cloud chemistry turned off in the simulation, also see the "chem_opt" parameter
	= 1	cloud chemistry turned on in the simulation, also see the "chem_opt" parameter
vertmix_onoff	= 0	vertical turbulent mixing turned off in the simulation (useful for debugging)
	= 1	vertical turbulent mixing turned on in the simulation (default)

chem_conv_tr = 0	subgrid convective transport turned off in the simulation (if no parameterization is used or for debugging)
= 1	subgrid convective transport turned on in the simulation (default)
conv_tr_wetscav = 0	subgrid convective wet scavenging turned off in the simulation (if no parameterization is used or for debugging)
= 1	subgrid convective wet scavenging turned on in the simulation (default)
conv_tr_aqchem = 0	subgrid convective aqueous chemistry turned off in the simulation (if no parameterization is used or for debugging)
= 1	subgrid convective aqueous chemistry turned on in the simulation (default). Currently connected to "MADE" modal aerosol options.
have_bcs_chem = .false.	gets lateral boundary data from idealized profile specified in chemistry routines (use caution when setting as the name list variable is defined as a logical)
= .true.	gets lateral boundary data from wrfbdy data file (use caution when setting as the name list variable is defined as a logical)
have_bcs_tracer = .false.	does not use tracer lateral boundary data from wrfbdy data file (use caution when setting as the name list variable is defined as a logical)
= .true.	gets tracer lateral boundary data from wrfbdy data file for tracer species
aer_ra_feedback = 0	no feedback from the aerosols to the radiation schemes
= 1	feedback from the aerosols to the radiation schemes turned on, see also chem_opt parameter
chemdiag = 0	turns off chemical tendency diagnostics
= 1	turns on chemical tendency diagnostics for equation budget analysis
cam_mam_mode = 3	Number of MAM aerosol modes
cam_mam_nspec = 74	Number of MAM 3-bin aerosol species
CAM_MP_MAM_cpled	Option to allow users to run Morrison-Gettleman micrphysics with prescribed aerosols (using &physics namelist options accum_mode, aitken_mode and coarse_mode) with the RRTMG radiation scheme. The RRTMG scheme will still use prognostic aerosols. Default value is set to .true. so that both the Morrison-Gettleman microphysics and the RRTMG radiation scheme use prognostic aerosols.

In the physics name list, there are options that are directly related to the chemistry. These include the options related to the aerosol direct and indirect forcing ra_sw_physics, progn, and mp_physics. In addition there is a cumulus radition feedback option, cu_rad_feedback, as well as online/offline cumulus cloud time average option, cu_diag. These options will only work with the GF or the G3 scheme (cu_phys=3 or 5). If the cu_rad_feedback is not turned on the radiation and photolysis schemes will not "see" parameterized clouds. If cu_diag is not turned on the time average cumulus cloud arrays will not be computed. These options will only work with WRF-Chem.

cu_rad_feedback	= .false.	no feedback from the parameterized convection to the atmospheric radiation and the photolysis schemes. (Use caution when setting as the name list variable is defined as a logical.)
	= .true.	feedback from the parameterized convection to the radiation schemes turned on. (Use caution when setting as the name list variable is defined as a logical)
cu_diag	= 0	turns off time average cumulus cloud
	= 1	turns on time average cumulus clouds
progn	= 0	turns off prognostic cloud droplet number in the Lin et al. and Morrison microphysics
	= 1	prognostic cloud droplet number included in the Lin et al. and Morrison microphysics scheme. This effectively turns the Lin et al. scheme into a second-moment microphysical scheme. If set with chem._opt=0 a default-prescribed aerosol concentration is used.
mp_physics	= 11	CAM5 Morrison-Gettleman scheme to be used with MAM chemistry
cu_physics	= 7	CAM5 Zhang-McFarlane scheme to be used with MAM chemistry
bl_pbl_physics	= 9	CAM5 UW PBL scheme to be used with CAM-MAM chemistry
shcu_physics	= 2	CAM5 UW shallow cumulus schemeto be used with CAM-MAM chemistry
accum_mode	= 1.e9	Background mass mixing ration for accumulation mode used with CAM_MP_MAM_cpled = .false.
aitken_mode	= 3.e8	Background mass mixing ration for Aitken mode used with CAM_MP_MAM_cpled = .false.
coarse_mode	= 2.e5	Background mass mixing ration for coarse mode used with CAM_MP_MAM_cpled = .false.

In the time_control name list there are options that are directly related to the chemistry, these include the options related to the reading of the various emissions data through the WRF auxiliary input ports and the methodology to read and write data files.

auxinput5_interval = 3600	input time interval for anthropogenic-emissions data. Typical settings are hourly for NEI emissions and monthly for the RETRO/EDGAR data
auxinput6_interval =	input time interval for biogenic-emissions data. Typically biogenic emissions are static fields and this setting is not used
auxinput7_interval =	input time interval for biomass burning (wildfire)-emissions data. For forecasts the wildfire emissions are often static fields and this setting is not used. For retrospective simulations the data can be updated according to the availability of additional fire information.
auxinput8_interval =	input time interval for GOCART background fields. Typically for

	forecasts the monthly background data are static fields and this setting is not used.
io_form_auxinput5 = 2	anthropogenic-emissions input (wrfchemi_00z_d01 and wrfchemi_12z_d01) data format is WRF netCDF
= 11	parallel netCDF
io_form_auxinput6 = 2	biogenic-emissions input (wrfbioemi_d01) data format is WRF netCDF. Can be used if bio_emiss_opt > 1
= 11	parallel netCDF. Can be used if bio_emiss_opt > 1
io_form_auxinput7 = 2	biomass burning-emissions input (wrffirechemi_d01) data format is WRF netCDF
= 11	parallel netCDF
io_form_auxinput8 = 2	GOCART background emissions input (wrf_gocat_bg_d01) data format is WRF netCDF
io_form_auxinput12 = 2	set to use previous simulation data to initialize chemistry (wrf_chem_input_d01). The data format is WRF netCDF
= 11	Parallel netCDF
io_form_auxinput13 = 2	Volcanic ash emissions input (wrfchemv_d01) data format is WRF netCDF. Can be used if emiss_opt_vol > 1
= 11	parallel netCDF. Can be used if emiss_opt_vol > 1
io_form_auxinput14 = 2	aircraft emissions input data format is WRF netCDF.
= 11	parallel netCDF.
io_form_auxinput15 = 2	CO_2 or GHG emissions input data format is WRF netCDF. Can be used if chem_opt = 16 or 17.
= 11	parallel netCDF. Can be used if chem_opt = 16 or 17.

4.3.1 Running with only dust aerosols

The WRF-Chem code is able to predict dust transport along with the meteorology. To run with only dust, you should have obtained several input data files for the WRF Preprocessor System (WPS). These files are the dust related fields (erosion factor, clay fraction, sand fraction) that are included in the WPS GEOG directory and the GEOGRIB.TBL_ARW_CHEM table file. The files are available for download if for some reason they were not included with your WRF WPS at:

ftp://aftp.fsl.noaa.gov/divisions/taq/dust_emissions_v3.3

After downloading the files and placing them in the correct WPS directories one needs to link the GEOGRIB table to GEOGRIB.TBL_ARW_CHEM. The WRF WPS can then be run so that the dust erosion fields will be included the geogrib output and subsequently included in the meteorology input data files. With the dust erosion data now in the input files WRF model can be run using the dust only name list settings (chem_opt=401). Be sure when running with the dust only option that the other chemistry name list settings (e.g., gaschem_onoff, phot_opt, gas_drydep_opt, etc.) are turned off and the dust_opt option is set to 1 or 3.

4.3.2 Running with direct effect

Shortwave radiative feedbacks or what is known as the direct effect is included with the running of chemistry. To turn on the radiative feedbacks in your simulation you should select either the RRTMG radiation schemes, or the Goddard shortwave scheme and turn on aer_ra_feedback (aer_ra_feedback=1). With these options selected the aerosol shading will be active and one can select an aerosol compostition assumption for the Mie radiation calculation using aer_op_opt. Another namelist option related to radiation that is typically used in a simulation is cu_rad_feedback. When turned on (cu_rad_feedback = .true.) the shortwave and photolysis schemes will include the effects of unresolved clouds in the simulation. Otherwise, the simulation could have a grid cell containing a strong precipitating thunderstorm (parameterized instead of resolved precipitation) but the surface incident radiation and photolysis calculations will produce a result for an environment is totally cloud free.

4.3.3 Running with indirect effect

There are several chemistry options that include the indirect effect and each of these options contain aqueous phase chemistry (e.g., RADM2SORG_AQ, RACMSORG_AQ, CBMZ_MOSIAC_4BIN_AQ, CBMZ_MOSAIC_8BIN_AQ, etc.). It has been assumed by the developers that if a user chooses to run with includes aqeuous phase chemistry, then they also choose to be running with the indirect effect (chemistry-microphysics interactions). If you do not want to include the indirect effect then one must either include a prescribed climatological aerosol distribution (e.g., Gustafson et al., 2007) or choose a chemistry option that does not include aqueous phase chemistry.

To run with indirect effect on, one should turn on the aerosol direct effect (aer_rad_feedback = 1 and aer_op_opt > 0). Next the user needs to select a double microphysics scheme; either Lin et al. or the Morrison microphysics schemes are the current possible choices. Next turn on the prognostic number density option (progn=1) in the physics namelist to make the Lin et al. scheme double moment as well as communicate the desire to run indirect effect to other microphysics schemes. Finally, turn on the wet scavenging and cloud chemistry options (wetscav_onoff=1; cldchem_onoff=1).

4.3.4 Tracers running with chemistry

The WRF-Chem code is now able to predict chemical tracers alongside reactive chemistry. **This tracer option is set in the namelist.input under the dynamics name list and not the chemistry name list.** This will allow a user to run WRF-Chem with chemistry *and* tracers simultaneously. To run with tracer edit your namelist.input file and add the following under the dynamics name list section:

tracer_opt	= 0	no tracers
	= 1	smoke tracer which must run with biomass burning
	= 2	lateral boundaries, stratospheric, boundary layer, and surface

		tracers
	= 3	same as tracer_opt=2 but surface tracer is replaced by the biomass burning tracer
	= 4	same as as tracer_opt=2 with the addition of a Lightning-NOx (LNOx) tracer, so must have the lightning NOx parameterization turned on (see Appendix E)
tracer_adv_opt	= 0	uses positive definite advection for tracers
	= 1	uses positive definite and monotonic advection for tracers. (Recommended)

The biomass-burning tracer (ppmv) obtains the carbon monoxide (CO) emissions from the biomass-burning-emissions input and provides this data as a tracer. Unlike the reactive species emitted from biomass-burning, the tracer experiences passive transport. When activating the tracer species using the tracer_opt name list option a pair of tracers is released in the run. The first tracer is considered completely passive, while the other has a first-order decay with a one-day lifetime. The lateral boundary data for each tracer sets the tracer concentration to a value of 1 and is advected into the model domain during the simulation. The stratosphere tracer is set to 1 above a specified minimum temperature at this time, but an update to using the World Meteorological Organization (WMO) tropopause definition is planned. The boundary layer tracer is set to 1 below the PBL height. And finally, the surface tracer is set to 1 at the lowest model level (k=1).

When setting tracer_opt=4 there will also be a pair of tracers produced for lightning-NOx (LNOx). The first tracer tracks NO produced from intra-cloud lightning; the second tracer tracks NO produced from cloud-to-ground lightning.

4.3.5 Considerations when running with CAM-MAM chemistry

Starting with version 3.5 of the WRF-chem model, the CAM5 micrphysics and MAM aerosol schemes has been made available. The MAM aerosol scheme, short for Modal Aerosol Model, is either a 7-mode and 3-mode modal aerosol scheme (Liu et al., 2012) derived from the Community Atmosphere Model (CAM), a component of the CESM climate model. The MAM scheme provides internally mixed representations of number concentration and mass for Aitkin, accumulation, and coarse aerosol modes. At this time the MAM is coupled only with CBM-Z photochemistry within WRF-Chem. In addition to MAM, the microphysics scheme from CAM has been ported to the WRF model. This scheme represents stratiform microphysical processes through a prognostic, two-moment formulation following the original parameterization of Morrison and Gettelman (2008). It should be noted that the CAM-MAM scheme (chem_opt=503) was extensively tested with the CAM physics inside WRF (CAMMGMP, CAMUWPBL, CAMZM, CAMUWSHCU, and RRTMG). The CAM physics options as well as the MAM chemistry could run with different combinations of the pre-existing physics and chemistry parameterizations in WRF, however, it is not recommended due to the lack of evaluation. Runs not using the full CAM-MAM package options should be examined by the user to ensure accuracy or whether the results contain numerical artifacts. In addition,

the user could encounter warning and error messages when running MAM chemistry independent of CAM microphysics as this is not fully tested and the model could be running in an unsupported configuration.

When running without chemistry, the CAM microphysics scheme (Morrison and Gettelman microphysics; Morrison and Gettelman, 2008) requires TKE to be computed in oder for the scheme to function properly, so it must be used with PBL a scheme that produces TKE (e.g., UW PBL or MYJ). This scheme also uses outputs from Zhang-McFarlane cumulus scheme and the UW shallow cumulus schemes as sources of input data (Zhang and McFarlane, 1995). Care must be taken as these fields are are set to zero when Zhang-McFarlane cumulus scheme and the UW shallow cumulus scheme are not in use and could result in run time errors. It is recommend that one use the CAM microphysics with the complete CAM physics suite (the UW shallow cumulus, Zhang-MacFarlane deep cumulus the UW PBL) when running the model to avoid encountering a run-time error.

When running the CAM physics suite (Morrison and Gettelman microphysics, UW shallow cumulus, Zhang-MacFarlane deep cumulus and UW PBL) with chemistry, it is recommended that the user can select from the four MAM aerosol packages. The CAM microphysics suite has not been tested with the other chemisry packages and could result in run error. If however, one wanted to test the UW PBL scheme with other chemistry options, this PBL scheme should not produce run time errors as it is an independent package. It should also be noted that the CAM microphysics in WRF does not include the full CAM5 macrophysics treatments. For this model implementation a simplified version of CAM5 macrophysics is incorporated in the CAM microphysics driver which aids in computing the CAM fractional clouds as opposed to pre-existing WRF cloud fractions (values between 0 and 1). The simplified cloud fraction inside WRF's CAM scheme uses the same formulation to calculate convective cloud fraction, and liquid and ice cloud fraction for stratiform clouds.

4.4 Typical choices for name list options

The addition of chemistry to WRF is making the choice of runtime configuration options much more complicated than for the meteorological version of WRF. Not all chemistry options are interchangeable with each other (e.g. not every chemical mechanism will work with every available aerosol module), not all physics options will work with all chemistry options. The name list description in the previous sections gives the user an idea of what physics options have to be chosen when applying the modeling system to study the aerosol direct and indirect effect. Work is in progress to extend the list of radiation and microphysics routines that will work with the aerosol routines. Work is also in progress to generalize the aerosol direct/indirect effect with respect to all available aerosol modules (e.g. allowing GOCART routines to interact with the atmospheric radiation schemes and the photolysis routines as well as allowing the full indirect effect for the modal aerosol scheme).

Even for very simplistic chemical setups seemingly small changes in the name list, options can cause large differences in the results. For real-time and research applications, we commonly use:

chem_adv_opt = 2
moist_adv_opt=2
scalar_adv_opt=2
tke_adv_opt=2
diff_6th_opt = 0

The above options should always be used when running chemistry simulations. The WRF advection scheme has the tendency to overshoot and produce locally unrealistically low values (referred to at times as "digging holes") if those options are not turned on. This "digging" is stronger with stronger gradients like those found where there are high emission rates.

cu_phys = 3 or 5
cugd_avedx=1
cu_rad_feedback=.true
chem_conv_tr = 1

The above options should be used if a convective parameterization is desired. The option chem_conv_tr will work with any other parameterization. However, cu_rad_feedback will only work with cu_phys=3 or 5. The latter option ensures that areas with convective precipitation will be seen by the atmospheric radiation scheme and the photolysis scheme. Not using any of the above convection-related options (chem_conv_tr=0) will underestimate the transport out of the boundary layer significantly. Setting false the cu_rad-feedback option will lead to photolysis rates that are unaffected by convection (too high), as well as skin and surface temperatures that are too warm. The cugd_avedx parameter is used by cu_phys=5 (G3 scheme) and should be set to one (1), except for forecasts high resolution of dx larger than 2km, but smaller than 10km. It will turn on subsidence spreading over neighboring grid points from the convective parameterization. In that case, set cugd_avedx=3 and cu_phys = 5. Other values are currently not allowed:

sf_sfclay_physics = 1
sf_surface_physics=2
bl_pbl_physics =1

The choice of the PBL physics is the most contested. It might depend strongly on the users own preferences. The user must keep in mind that results can differ significantly depending on this choice. The YSU scheme will lead to the deepest boundary layers when using the above choices (1-2-1). The user may also go to 2-2-2, using the MYJ scheme. There is no sure way of telling which will work better. We also sometimes choose the RUC soil parameterization (2-3-2) in combination with either YSU or MYJ scheme. This may work fine when the input conditions come from the RUC. The question of what modeling system the input and boundary conditions come from (such as

GFS, NAM, ECMWF, etc.) and what type of physics are used in that modeling system can play a role too in determining the choice of PBL physics. The user may want to try to be consistent with the larger scale model, or choose the larger scale model based on his preferred choice of physics options – if possible. An additional consideration here is also the availability of an initial cloud analysis. This is available WRF-based Rapid Refresh (RAP) and may be essential in reducing spin-up. New PBL parameterizations are now also available. These show great promise. You may try the MYNN scheme. It was tested successfully with chemistry:

mp_zero_out = 2

We always choose this option if not using positive definite advection. It ensures that hydrometeor mixing ratios are not allowed to grow smaller than a threshold value (mp_zero_out_thresh), in particular qv as well as other moisture-mixing ratios will never go negative.

chem_dt = 0 [sets chem_dt = time_step; remember that the units are in minutes]

If you are using chem_opt=1 or 2, we advise to use the timestep as is used by the meteorological part of the model. That is, set chem._dt = 0 and the chemistry will use the same time step as used by the meteorology dynamics part of the model. You can choose larger time steps for any of the other options of chem_opt, but may want compare your results to a control simulation with chem._dt=0.

4.5 Input fields for chemical constituents

Unless chemical fields are available from a modeling system (global model, larger scale model, or even another WRF-Chem run), an idealized vertical profile for each chemical species is provided to start the model simulation. This vertical profile, obtained when the model is initialized with chem_in_opt set equal to zero "0" in the namelist.input, is based upon northern hemispheric, mid-latitude, clean environment conditions. If modifications are required, the routine module_input_chem._data can be modified to produce the desired initial conditions. Note that if the initial fields are modified, the boundary conditions will probably also need to be modified (also located in module_input_chem_data).

The idealized profile is obtained from climatology in the routine module_input_chem._data with data based upon results from the NALROM numerical chemistry model. The profile is declared globally inside the routine so that the lateral boundary conditions for a chemistry simulation may also be derived from this idealized profile. For ease of use, please note that in this module, the variable "iref" is the reference index, and "fracref" is the reference fraction corresponding to iref. For example, the species number 1 for a WRF-Chem simulation is SO_2. The first reference index for the idealized profile, iref(1), is set to the number 12, indicating that SO_2 is taken from the 12^{th} species in the input data table. Not all chemical species match up so cleanly. For example, the NALROM model calculates its chemistry using lumped OX

(where OX = O3 + NO2 + HNO3 + ...) and a lumped NOX is obtained from (NOX = NO + NO2 + NO3 + 2N2O5 + HO2NO2 + HONO). However, the RADM2 chemical mechanism strictly uses O3, and NOx is a combination of NO + NO2 only. Therefore, fractions of chemical species based upon the values of fracref are used to separate the lumped chemical species into the chemical species used by the RADM2 chemical mechanism.

Short-lived species are initialized to steady-state equilibrium - since they are short-lived. The short-lived species within a lumped category (Ox, NOx, or NO3+N2O5 in our case) would be renormalized to the lumped class after the steady-state equilibrium concentrations are determined.

The following is the list of long-lived species provided by the NALROM chemistry model:

NAMEL(1)	OX
NAMEL(2)	NOX
NAMEL(3)	HNO3
NAMEL(4)	H2O2
NAMEL(5)	CH3OOH
NAMEL(6)	CO
NAMEL(7)	ISOPRENE
NAMEL(8)	CH2O
NAMEL(9)	CH3CHO
NAMEL(10)	PAN
NAMEL(11)	OTHER ALKA
NAMEL(12)	SO2
NAMEL(13)	BUTANE
NAMEL(14)	ETHENE
NAMEL(15)	PROPENE
NAMEL(16)	PPN
NAMEL(17)	MEK
NAMEL(18)	RCHO
NAMEL(19)	SO4
NAMEL(20)	MVK
NAMEL(21)	MACR
NAMEL(22)	HAC
NAMEL(23)	MGLY
NAMEL(24)	HPAN
NAMEL(25)	MPAN
NAMEL(26)	PROPANE
NAMEL(27)	ACETYLENE
NAMEL(28)	OH
NAMEL(29)	HO2
NAMEL(30)	NO3 + N2O5
NAMEL(31)	HO2NO2

NAMEL(32) SUM RO2
NAMEL(33) OZONE
NAMEL(34) NOX

4.6 Using chemical boundary conditions from other modeling systems

At this time, tools to provide data for the lateral boundary have been provided by the user community. Most of these tools are still under development and are supported by the individual groups. Each of these tools are designed to provide larger scale data from models other than WRF as boundary and initial conditions to the WRF-Chem simulations.

4.6.1 The wrfchembc utility

One utility program to produce chemical lateral boundary conditions, available from NOAA/ESRL, is called wrfchembc. This program currently works with data – for a selected number of species - from the MPI-MATCH and RAQMS global chemistry models. You can download the latest version of the code from the ESRL ftp site. For example, the latest code might be named

ftp://aftp.fsl.noaa.gov/divisions/taq/Boundary/wrfchemv2.2_bcond_code_09Apr07.tar

You can then modify the Makefile to use your desired compile options and compile to generate the wrfchembc executable. You must also modify the wrfchembc_namelist.input file to have the correct data directories and species added to the wrfbdy file.

Run the wrfchembc program after real.exe and before wrf.exe to add the global model data to the lateral boundary data file (wrfbdy_d01). In addition, before running wrf.exe, modify the namelist.input to set have_bcs_chem = .true.

4.6.2 The mozbc utility

Another tool is provided by NCAR/ACD and is designed to create time-varying chemical boundary conditions from the MOZART global model to a WRF-Chem simulation. The mozbc utility is a single cpu code that maps species concentrations from MOZART datasets to WRF-Chem concentrations for initial condition and boundary condition datasets. The utility is setup for MOZART species concentrations to be in volume mixing ratio and converts the species units to WRF-Chem depending on whether it is a gas or aerosol. The mozbc utility allows for a versatile mapping to each WRF chemical species from MOZART species including multiple with choices for:

- An individual weight factor per MOZART species; and
- An overall conversion factor per WRF-Chem species.

The mozbc utility requires users to have a WRF-Chem initial condition file (wrfinput_d<domain>) for each domain of interest and/or a WRF-Chem boundary condition file (wrfbdy_d01) for the first WRF-Chem domain. The Mozart datasets are interpolated in space (bilinearly in longitude, longitude and linearly in pressure), **but not in time**. Therefore, users need to ensure that the times in the MOZART and WRF-Chem files are matching for the period of interest. Otherwise, if a non-matching time is found, the mozbc will abort the run with an error statement.

4.7 VPRM and Greenhouse Gas tracer namelist options

There are several chemistry namelist options that are used only by the CO_2 tracer and Greenhouse Gas tracer chemistry options. These namelist options are:

vprm_opt	This option allows a user to select a parameter set for the VPRM model. There are three sets of parameters - "VPRM_TABLE_US", "VPRM_TABLE_EUROPE" and "VPRM_TABLE_TROPICS" (included in chem/chemics_init.F) used for different regions. Users may need to build own parameter sets for the domain and time period of interest. (default is "VPRM_param_US")
wpeat	Used to specify the scaling factor for the CH_4 wetland emissions from peatlands. It indicates the fraction of heterotrophic respiration that is considered to be CH_4 emissions. (default is 0.05)
wflood	Used to specify the scaling factor for the CH_4 wetland emissions from floodplains. Weighting between peat and floodplain wetlands depends on the mean annual temperature. Users may need to calibrate the Kaplan wetland inventory with observations first and then adjust both scaling factors. (default is 0.19)
term_opt	user to select the parameter set for the calculation of the termite emissions. Two sets of parameters are included: "CH4_termite_NW" to be used for the American continent and Australia and "CH4_termite_OW" for Europe, Asia, and Africa. Both are included in chem/chemics_init.F. (default is "CH4_termite_NW")
wflood	Used to specify the scaling factor for the CH4 wetland emissions from floodplains. Weighting between peat and floodplain wetlands depends on the mean annual temperature. Users may need to calibrate the Kaplan wetland inventory with observations first and then adjust both scaling factors. (default is 0.19)

4.8 Making a nested domain WRF-Chem simulation

To make a nested domain run one should first produce wrfinput files for both domains following Chapter 4 of WRF Users Guide. Like the single domain WRF-Chem simulations, it is probably best to start by making a nested domain weather forecast

(Chapter 4 of WRF Users Guide). After the nested meteorology only simulation is functioning correctly, then move on to running with chemistry included in the simulation.

Once the input files are produced the user can generate the emissions files for both domains using their program of choice (e.g., the emiss_v03.F program discussed in section 3 of Quick Step Guide, Chapter 2 of the User's Guide). File anthropogenic emissions file names will be differentiated by the domain (ie., wrfem_00to12z_d01 and wrfem_00to12z_d02).

The convert_emiss.exe program is not currently designed to read the namelist.input file and generate the nested domain emissions files. Therefore, run the conversion program treating the nested domain as if it was actually the mother domain. That is, for each domain you will run convert_emiss.exe using settings for a single domain in your namelist.input file. More specifically, follow the description in section 3 to generate wrfchemi_d01 for the coarse domain, and move it to a safe place by changing its name. Change the namelist.input file, moving the nested information to the mother domain column. Move the met wrfinput_d02 to wrfinput_d01, link the output from emisv03 (for the nested domain) to the required filenames, and then run convert_emiss. Finally, move the resulting wrfchemi_d01 to wrfchemi_d02.

When running wrf.exe with more than one domain (e.g., 2-way nested simulation), nearly every chemistry name list option needs to be set for each domain. A user should always examine the Registry/registry.chem file and check each of the chemistry name list variables. Those variables that are dimensioned max_domains need to be set for each domain. The following example shows how the chemistry name list variables might be configured for a simulation using more than one domain.

```
&chem
kemit                 = 19,
chem_opt              = 301, 301,
bioemdt               = 30, 30,
photdt                = 30, 30,
chemdt                = 2.0, 0.66666,
io_style_emissions    = 1,
emiss_opt             = 5, 5,
emiss_opt_vol         = 0, 0,
chem_in_opt           = 1, 1,
phot_opt              = 1, 1,
gas_drydep_opt        = 1, 1,
aer_drydep_opt        = 1, 1,
bio_emiss_opt         = 1, 1,
dust_opt              = 0,
depo_fact             = 0.25, 0.25,
dmsemis_opt           = 0,
seas_opt              = 0,
```

```
gas_bc_opt                          = 1, 1,
gas_ic_opt                          = 1, 1,
aer_bc_opt                          = 1, 1,
aer_ic_opt                          = 1, 1,
gaschem_onoff                       = 1, 1,
aerchem_onoff                       = 1, 1,
wetscav_onoff                       = 0, 0,
cldchem_onoff                       = 0, 0,
vertmix_onoff                       = 1, 1,
chem_conv_tr                        = 1, 1,
conv_tr_wetscav                     = 1, 1,
conv_tr_aqchem                      = 1, 1,
biomass_burn_opt                    = 1, 0,
plumerisefire_frq                   = 30, 0,
aer_ra_feedback                     = 0, 0,
aer_op_opt                          = 0, 0,
have_bcs_chem                       = .false., .false.,
```

Chapter 5: Visualizing WRF-Chem Data files

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5.1 Introduction

The WRF modeling system has a number of visualization tools that are available to display data. Since the model output data is netCDF format, essentially any tool capable of displaying this data format can be used to display the WRF model data. Currently, NCAR supports four graphical tool packages (NCL, RIP4, WRF-to-GrADS, and WRF-to-vis5d. A description of each of these tools is also available online at:

http://www.mmm.ucar.edu/wrf/users/graphics/WRF-post-processing.htm.

The WRF-Chem model, being part of the WRF modeling system, can likewise use any of the WRF netCDF visualization tools. A detailed description of all available visualization tools is beyond the scope of this User's Guide. Instead this chapter will discuss a few of the tools that are being used to examine WRF-Chem input and output files – ncdump, ncview and RIP. However, each user is encouraged to explore the multitude of netCDF visualization tools that are available and use the one(s) that are best suited to their needs.

5.2 The ncdump application

The ncdump utility is distributed by Unidata and installed with the netCDF library. This application is a netCDF file viewer that can be used to generate ASCII representation of the data. There are some limits to what this program can do with point (e.g., surface station) data, but there are more options available for examining array data. However, ncdump can be cumbersome when examining large volumes of array data. The Unidata web page

http://www.unidata.ucar.edu/software/netcdf/docs/ncdump-man-1.html,

contains a detailed description of the ncdump command and examples of its usage.

5.3 Using NCL scripts

NCL is among the many post-processing utilities to visualize WRF output. This section briefly describes a script that can be used to generate a plot of chemical species. For additional information about NCL, the reader is directed to Chapter 8 in the WRF Model User's Guide.

Following the NCL script examples, the following script has been generated to plot ozone for the 1 August 2000 at 0000 UTC. The user is required to set the date and run directory (direc) as well as the header for the file name (filnm) and field to be plotted in the script. The gas phase species can be converted to ppm from ppb for easier plotting and viewing. The script is as follows:

```
load "$NCARG_ROOT/lib/ncarg/nclscripts/csm/gsn_code.ncl"
load "$NCARG_ROOT/lib/ncarg/nclscripts/csm/gsn_csm.ncl"
load "$NCARG_ROOT/lib/ncarg/nclscripts/wrf/WRF_contributed.ncl"

begin

; read in wrfout file

   date = "08-01_00"

   direc = "./"

; filename=filnm

   filnm = addfile(direc+"wrfout_d01_2000-"+date+":00:00.nc","r")

; extract field to be plotted from file

   ozone = filnm->o3

; scale by 1000 (convert ppm to ppb)
   ozone = ozone*1000.
   ozone@units = "ppbv"

;=================================================================
; set up plotting parameters

; creating 2 workstations to plot both to screen (x11) and to a pdf file
  wks = gsn_open_wks("x11","ozone_lev50_"+date)
  wks_2 = gsn_open_wks("pdf","ozone_lev50_"+date)
  gsn_define_colormap(wks,"WhViBlGrYeOrRe")    ; choose colormap for wks
  gsn_define_colormap(wks_2,"WhViBlGrYeOrRe")  ; choose colormap for wks_2

; assign plotting resources

  res = True
  res@gsnMaximize     = True
```

```
  res@gsnSpreadColors = True               ; use full range of color map
  res@cnFillOn        = True               ; turn on color fill
  res@cnLinesOn       = False              ; turn off contour lines
  res@cnLineLabelsOn  = False              ; turn off contour line labels
  res@cnLevelSelectionMode = "ManualLevels"  ; set explicit contour levels
  res@cnMinLevelValF = 60
  res@cnMaxLevelValF = 110
  res@cnLevelSpacingF = 5
;
  res@tiMainString = "OZONE CONC. AT "+date+"UTC"

;=================================================================

; use WRF_contributed procedure to set map resources

   WRF_map_c(filnm,res,0)

; define lat, lon

   ozone@lat2d = filnm->XLAT(0,:,:)
   ozone@lon2d = filnm->XLONG(0,:,:)
;
; plot ozone at the lowest level

   plot = gsn_csm_contour_map(wks,ozone(0,0,:,:),res)
   plotpdf = gsn_csm_contour_map(wks_2,ozone(0,0,:,:),res)

end
```

By issuing the ncl execution command

ncl <script name>

The contour plot showing ozone concentration over the domain is generated (Figure 5.1).

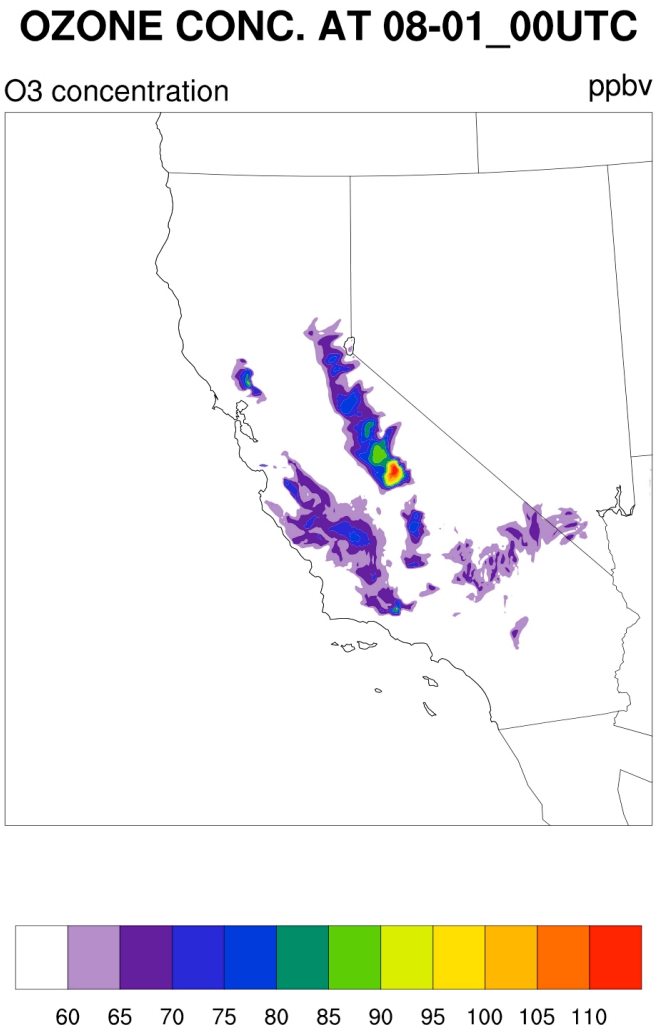

Fig. 5.1 A sample of a color-filled contour plot generated using the NCL script. The colored regions represent locations in which the surface ozone concentration (ppbv) is in the range indicated by the color bar shown at the bottom of the figure.

5.4 The ncview application

The Ncview application is a visual browser for netCDF data developed by David W. Pierce of the Scripps Institution of Oceanography. Ncview reads the wrfout files (also all input files, including the emissions) directly using the simple command ">ncview wrfout…". This makes it a very useful tool for a quick look analysis or diagnosis of a problem with the model run, including problems with any of the input files. Ncview installs onto UNIX platforms under X11 and provides an easy, push-button method to examine the contents of a netCDF file (Fig. 5.2). When looking at the data you can change the color maps, invert the data, generate line plots, etc. In addition, if the file contains a time series, Ncview permits simple animation of the data. An additional information program as well as a link to download the source code is available online at:

http://meteora.ucsd.edu/~pierce/ncview_home_page.html.

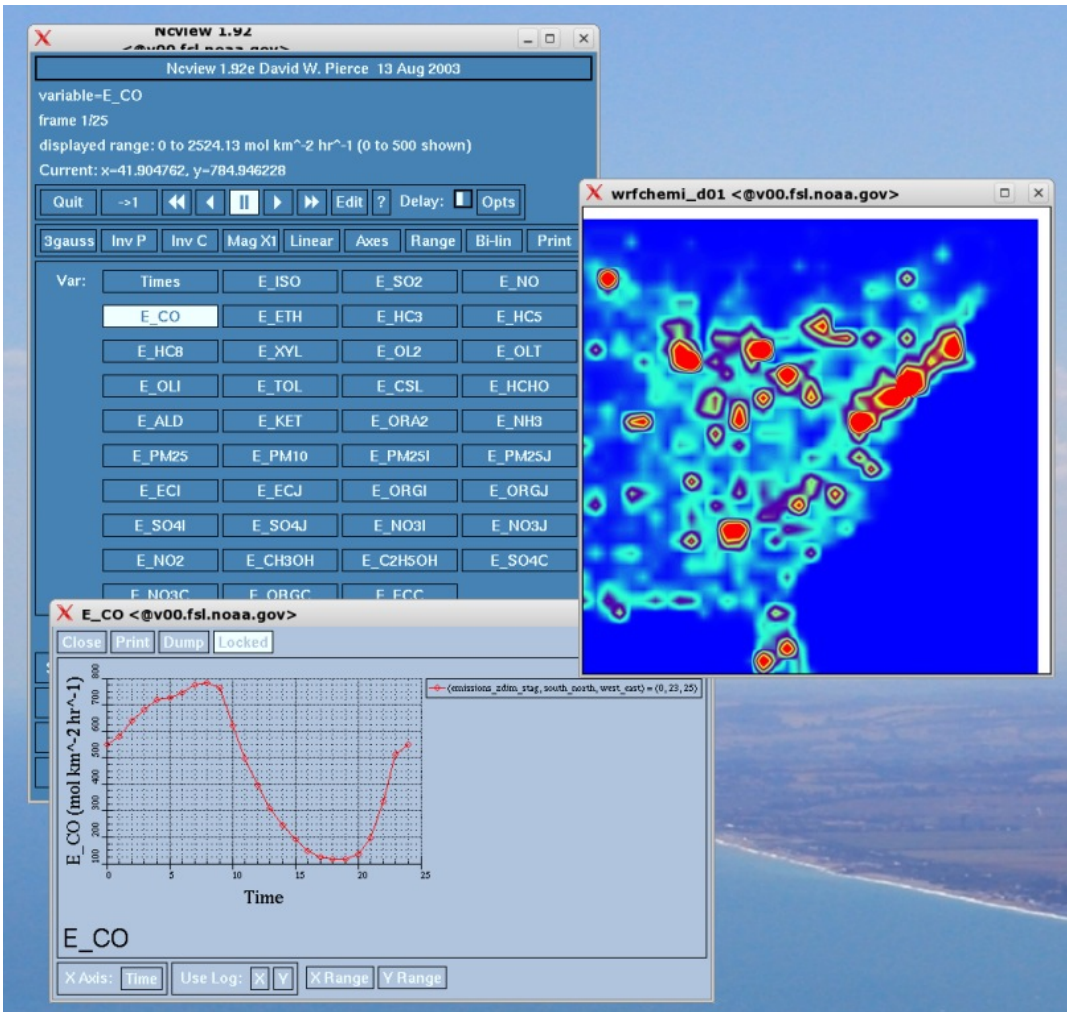

Fig. 5.2 A screen-capture image showing how the Ncview user interface allows the user to examine the WRF-Chem emissions-input data file. The color image shows the surface emissions for carbon monoxide and the plot shows the temporal evolution of the surface CO emissions at a single point.

5.5 The RIP application

5.5.1 Downloading and installing the RIP program

The FORTAN program RIP (Read/Interpolate/Plot) invokes NCAR Graphics routines to produce two-dimensional images from gridded numerical model data. Originally designed to work with the PSU/NCAR Mesoscale Model (*i.e.,* MM5), it has been modified by Mark Stoelinga to work with the WRF model. RIP is officially supported by the National Center for Atmospheric Research (NCAR) and functions on

UNIX systems that have a FORTRAN 77/90 compiler and the NCAR Graphics Library. Documentation regarding the RIP program is available online at:

http://www.mmm.ucar.edu/wrf/users/docs/ripug.htm.

RIP is not fully interactive, but instead it requires the user to specify the desired plots through a formatted text file. NCAR Graphics CGM files are created when the RIP program is executed and these files can be viewed with any one of several different metacode translator applications (*i.e.,* idt, ctrans). Additional plots or modification of any existing plots is accomplished through changing the formatted text file and re-executing the RIP program.

5.5.2 Pre-processing data from WRF-Chem

Before using RIP to plot WRF-Chem output, one first needs to specify the location of the RIP executable by setting the environmental variable RIP_ROOT. In c-shell syntax, if the RIP code is located in /home/username/RIP, the command is:

setenv RIP_ROOT /home/username/RIP.

After setting the RIP_ROOT environmental variable, the WRF-Chem data files need to be converted to data files having the format expected by the RIP program. The RIP data preprocessor program, or rip_dp, is used to accomplish this task. Like RIP, a formatted text file is needed to specify what operations are to be performed. The rip_dp input data file (named ripdp.in for example) might look similar to the following example:

```
&userin
 ptimes=0,-
72,3,ptimeunits='h',tacc=30.,discard='QGRAUP','Q2','T2','TH2','AC0','AC
O3','ALD','ANTHA','CANWAT','cor','CORN','COSALPHA','CSL','CU_CO_TEN','D
CB','DEP_VEL','dmap','E','ECI','E_ECI','orgaro1j','orgaro2j','orgaro1i'
,'orgaro2i','orgba1i','orgba1j','orgba2i','orgba2j','orgba3i','orgba3j'
,'orgba4i','orgba4j','orgole1i','orgole1j','orgpai','orgpaj','p25i','p2
5j','nh4ai','nh4aj','no3ai','no3aj','E_NH3','E_ORGI','E_SO2','ETH','EXC
H_H','GLW','GLY','GRDFLX','h2o2','hc3','hc5','hc8','hfx','hno3','hno4',
'ho','ho2','hono','ISLTYP','ISO','IVGTYP','KET','LANDMASK','LH','MGLY',
'MU','MUB','n2o5','nh3','nu0','ol2','olt','onit','op1','op2','paa','pan
','rtc','rte','SEAS','SFROFF','SH2O01','SH2O02','SH2O03','SH2O04','SINA
LPHA','tol','tpan','UDROFF','xyl',
 iexpandedout=1
 &end
```

In this file the number of hours (72), the time interval (3) and the arrays that are to be excluded from preprocessing are specified.

The command to run the rip_dp program might look like the following:

```
ripdp_wrf –n ripdp.in /Data/wrfplots all /WRFV3/test/em_real/wrfout_d01_2008-07-14_12:00:00
```

The execution of the rip_dp program will produce many small Rip data files. These files are located in the Data Directory and are named like the following files:

wrfplots_0000.00000_ALBEDO
wrfplots_0000.00000_V10
wrfplots_0000.00000_ALT
wrfplots_0000.00000_VEGFRA
wrfplots_0000.00000_TMN
wrfplots_0000.00000_SO2
…

5.5.3 Generating NCAR GKS plots using RIP

Before generating the NCAR graphics data files, the user needs to provide all of the specific details in RIP user input data file, rip.in. The first part of this data file consists of two name lists: the userin name list that holds the general input specifications and the trajcalc name list that controls the creation of trajectory plots. The second part of the rip.in file holds a specification table that controls the generation of the plot(s). The reader should examine the online RIP documentation for a more detailed explanation.

For the generation of a horizontal plot showing the fine particulate matter (PM2.5) and the horizontal winds at the surface and placed on a map of the simulation domain, the rip.in data file would look similar to the following:

```
 &userin
 idotitle=1,title='PM2.5 Level 1',titlecolor='def.foreground',
 ptimes=${hour},
 ptimeunits='h',tacc=180,timezone=-7,iusdaylightrule=1,
 iinittime=1,ivalidtime=1,inearesth=0,
 flmin=.09, frmax=.92, fbmin=.10, ftmax=.85,
 ntextq=0,ntextcd=0,fcoffset=0.0,
 idescriptive=1,icgmsplit=0,maxfld=10,itrajcalc=0,imakev5d=0
 &end
 &trajcalc
 rtim=15,ctim=6,dtfile=3600.,dttraj=600.,vctraj='s',
 xjtraj=95,90,85,80,75,70,65,80.6,80.6,80.6,80.6,80.6,80.6,
 yitraj=50,55,60,65,70,75,80,77,77,77,77,77,77,
 zktraj=.9,.9,.9,.9,.9,.9,.9,.99,.9,.8,.7,.6,.5,
 ihydrometeor=0
 &end
==========================================================================
--------------------    Plot Specification Table    --------------------
==========================================================================
feld=PM_2.5_DRY; ptyp=hc; vcor=s; levs=b1; cint=.5; cmth=fill;>
   smth=2;cosq=.0,violet,2.,dark.blue,4.,blue,6.,green,>
        8.,light.green,10.,dark.yellow,15.,yellow,>
        20.,red,30.,red.coral,40.,orange,50.,tan,>
        60.,light.gray,70.,med.gray,80.,black,100.,white
feld=uuu,vvv; ptyp=hv; nttl;vcmx=-1; colr=black;linw=2
feld=map; ptyp=hb
feld=tic; ptyp=hb
```

==========

Generation of a NCAR CGM data file is done by issuing the command:

${RIP_ROOT}/rip rip.in wrfplots

in the /Data directory. With the successful execution, a file named wrfplots.cgm is created. As mentioned previously, the CGM data file can be viewed using any of the CGM file viewers like ctrans. For example, to use ctrans to view the CGM file, issue the command:

${NCARG_ROOT}/bin/ctrans -d X11 wrfplots.cgm.

The product from executing this command will be an image like the one shown in Fig. 5.3.

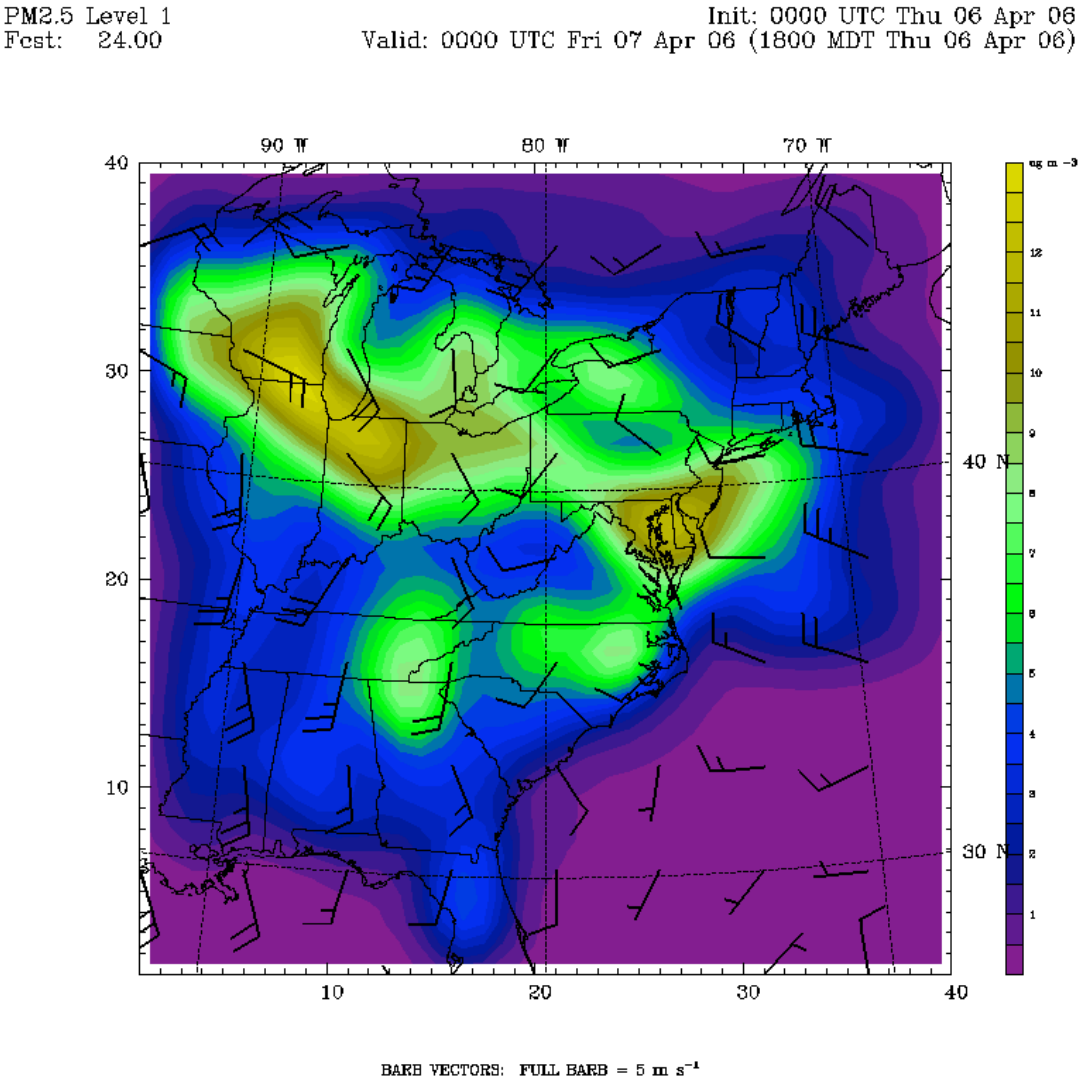

Fig. 5.3. An NCAR GKS figure produced using by the RIP visualization tool. The image shows the surface fine particulate matter (PM2.5) concentration (micrograms per cubic meter) and the horizontal surface winds (barbs).

With the successful visualizing of the results from a WRF-Chem simulation, one could add additional fields to plot by making additional RIP user-input data files for each individual plot, or modify the previous image specifications in a user-input data file. After modifying the user-input data file(s), you would only need to (re)create the NCAR CGM file(s).

Chapter 6: WRF-Chem KPP Coupler

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6.1 Introduction

Coupled state-of-the-art meteorology/chemistry models such as WRF-Chem typically include hundreds of reactions and dozens of chemical species. Solving the corresponding huge systems of ordinary differential equations requires highly efficient numerical integrators. In the case of hard-coded manually "tuned" solvers, even minor changes to the chemical mechanism, such as updating the mechanism by additional equations, often require recasting the equation system and, consequently, major revisions of the code. This procedure is both extremely time consuming and error prone.

In recent years, automatic code generation has become an appreciated and widely used tool to overcome these problems. The Kinetic PreProcessor (KPP) is a computer program which reads chemical equations and reaction rates from an ASCII input file provided by the user and writes the program code necessary to perform the numerical integration (Damian et al. 2002; Sandu et al. 2003; Sandu and Sander 2006). Computational efficiency is obtained by automatically reordering the equations in order to exploit the sparsity of the Jacobian. While still in a developmental stage, KPP Version 2.1 has been sucessfully implemented into WRF-Chem. Furthermore, a preprocessor for WRF-Chem has been developed that automatically generates the interface routines between the KPP-generated modules and WRF-Chem, based on entries from the WRF-Chem registry files and the KPP input files. This WRF-Chem-KPP coupler, WKC hereafter, is automatically executed during code compilation and considerably reduces the effort to add chemical compounds and/or reactions to existing chemical mechanisms. Likewise, the effort needed to construct new chemical mechanisms code has been greatly reduced due to the addition of KPP into WRF-Chem.

The WRF-Chem KPP Coupler, or WKC, was discussed by Salzmann and Lawrence (2006) at the WRF-User Workshop. The abstract is for the presentation is available with the KPP documentation in the WRF-Chem code (WRFV3/chem/KPP/documentation/abstr_wkc.pdf). A more complete set of

documentation for KPP (Kinetic PreProcessor) is also provided on line by Adrian Sandu at:

http://people.cs.vt.edu/ asandu/Software/Kpp/.

References for the KPP are Damian et al. (2002); Sandu et al. (2003); Sandu and Sander (2006) and it is requested that these references are cited when presenting results from the KPP generated code. KPP and WKC are distributed under the GNU General Public License (GPL). Constructive comments and suggestions regarding the coupler and/or this documentation are welcome. Only a limited number of all KPP features are available for use with WKC, but more features may be added in the future. In the remainder of this chapter, the WKC as implemented into the WRF-Chem model is described. Since the coupler has been only recently added to the WRF repository, it is possible that some design details could change based upon response from the WRF model developers as well as the WRF-Chem user community.

6.2 KPP requirements

KPP requires the UNIX tool programs flex, yacc, and sed to be installed on your system before compiling the code. Check with your system administrator if these programs are not installed. The path to the flex library (either libfl.a or libfl.sh) is specified by the environment variable FLEX_LIB_DIR. The default path for these libraries is assumed to be /usr/lib. If the library libfl.a (or libfl.sh) is not located in /usr/lib on your system, the variable FLEX_LIB_DIR should be set prior to compiling WRF-Chem. The C compiler is set by configure_kpp based on the settings in configure.wrf.

6.3 Compiling the WKC

The WKC, and therefore KPP as well, are compiled and executed automatically when WRF-Chem is compiled with the WRF_KPP environmental variable set (setenv WRF_KPP 1). The WKC copies the KPP generated code to the WRFV3/chem directory and automatically modifies the chemistry Makefile so that the KPP generated code is compiled and linked with the model. The KPP and WKC-generated modules in the chem directory contain the string “kpp” in their file names. Running the clean script removes these modules.

6.4 Implementing chemical mechanisms with WKC

KPP files for chemical mechanisms that have already been implemented with WKC are located in subdirectories of WRFV3/chem/KPP/mechanisms. The corresponding packages are declared in the WRFV3/Registry/registry.chem file and contain the suffix “kpp” in their name. In order to use one of these mechanisms with WRF-Chem, set the chem_opt variable in the namelist.input file to the appropriate value. The following mechanisms are currently available:

- RACM/SORGAM

- RACM (Stockwell et al. 1997)
- RACM-MIM (Geiger et al. 2003)
- RACM/SORGAM

These WKC implemented mechanisms have chem_opt greater than 100. The methodology for implementing additional mechanism(s) using KPP is discussed later in this chapter.

6.5 Layout of WKC

WKC reads KPP species input files with suffix .spc and the file Registry/registry.chem and automatically generates the Fortran 90 interface routines between WRF-Chem and the KPP generated code (see Fig. 6.1). It is in part based on the WRF registry mechanism. The WKC related files are located in the chem/KPP directory. This directory contains:

- a subdirectory mechanisms which holds directories with KPP input files for different mechanisms;
- a compile and a clean script for WKC (which are executed from the WRF-Chem compile script);
- a version of KPP v2.1 in the kpp subdirectory. This version of KPP was adapted to produce code which can directly be used with WRF-Chem (using the #WRF Conform option in the .kpp file);
- the source code of WKC in the util/wkc subdirectory;
- module wkpp_constants.F which allows to specify input to kpp such as RTOL and ATOL (likely to be extended in the future); and
- a subdirectory inc containing files which are included during compile time (using "#include" statements). The files in chem/KPP/incare not removed by the WKC clean script. Their purpose is to allow user modifications to WKC generated code.

At the heart of WKC is the routine gen kpp.c that is located in the util/wkc directory.

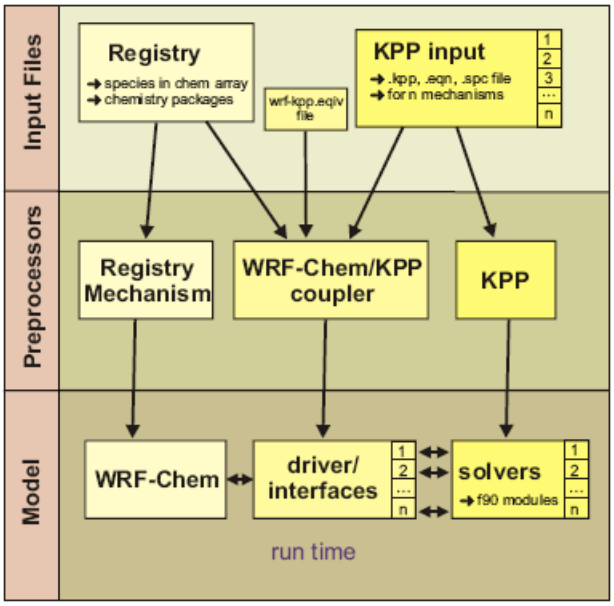

Fig. 6.1. Schematic showing the flow structure of KPP in the WRF-Chem model. Flowing down from the top, the Registry and KPP input data files (ASCII) are preprocessed into Fortran 90 and C code which is coupled to the WRF-Chem solvers.

6.6 Code produced by WKC, user Modifications

The code produced by WKC is called from the chem driver (see schematic call tree in Fig. 6.2). Since parts of the code are generated automatically, manual changes will be lost when recompiling WRF-Chem (as indicated by a warning in the header of the corresponding files). There are, however, a number of "#INCLUDE" preprocessor statements in the WKC generated code. The files included (in the .f files) are located in the chem/KPP/inc directory. These files are not removed by the clean script and can be used to inline user supplied code. In case this should not be enough, there are two ways to edit automatically generated files permanently: The files can either be renamed in such a way that they won't be removed by the clean kpp script; or the C code which generated the files (either KPP or WKC) can be edited. The latter is generally the better solution. However, the method of using include files in the chem/KPP/inc directory is strongly recommended.

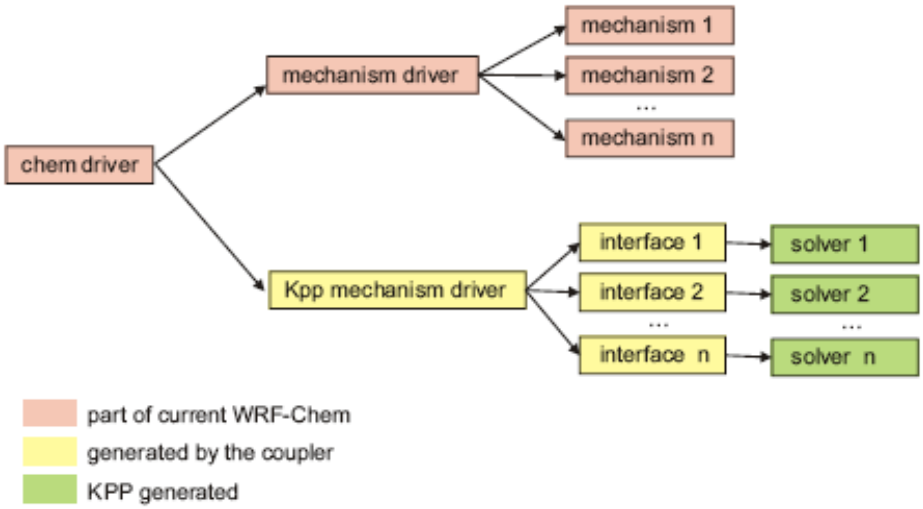

Figure 6.2: Schematic of the KPP call tree. Here the chem_driver routine in WRF-Chem calls a separate mechanism driver for each chemical mechanism implemented with KPP. This model configuration requires only one additional subroutine to be added to WRF-Chem so that the user can switch between the different implemented chemical mechanisms.

6.7 Available integrators

References for the chosen integrator after compiling WRF-Chem with KPP can be found in the chem directory in module kpp my mechanism Integrator.f90, where ‘‘my mechanism’’ refers to the chemical mechanism chosen in the WRF-Chem namelist. Currently, only Rosenbrock type integrators are available for the use with the WKC. More on the methodology to add additional integrators to the WKC will be discussed in a later section.

6.8 Adding mechanisms with WKC

When implementing new mechanisms, it is often necessary to calculate additional photolysis rates, include new emission datasets, specify initial and boundary conditions, calculate additional dry deposition rates, specify Henry’s law coefficients for soluble trace gases and carry them through the wet deposition routines, etc., in addition to the following steps.

The following basic steps are necessary in order to add a mechanism:

- edit the registry file Registry.EM_CHEM to
  - add species to the chem array structure (if necessary), and
  - add a package (a mechanism) with a name ending on “_kpp”, e.g., my_mechanism_kpp;

- provide input files my_mechanism.eqn, my_mechanism.spc, my_mechanism.kpp for KPP in a sub-directory of WRFV3/chem/KPP/mechanisms named after the package (i.e. my_mechanism, not my_mechanism_kpp); and
- optionally provide a file (my_mechanism_wrfkpp.equiv) for mapping variable names in WRF-Chem to variable names in KPP (e.g. HO to OH).

For additional examples, you can examine the chemical mechanisms that have already been implemented. You should note that when copying one of the directories in WRFV3/chem/KPP/mechanisms to another directory, it is necessary to change the name of #Model in the .kpp file and the names of the .eqn and the .spc file in the .def file. When introducing a "new" .kpp file you should set the #INTEGRATOR to an integrator contained in the directory WRFV3/chem/KPP/kpp/kpp-2.1/int/WRF_conform. For example, set

#INTEGRATOR WRF conform/rosenbrock

and add the line

#WRFCONFORM

to your new .kpp file. You should remember that not all KPP options are supported by the WKC. Also, the WKC is currently not able to handle comments in the .spc file!

6.9 Adapting KPP equation files

The process of adapting a KPP equation file for use with WRF-Chem involves renaming a few variables in the equation file:

	KPP equation file	Equation file units	Registry
Photolysis rate	J(Pj_no2)	s^{-1}	ph_no2
Temperature	TEMP	K	t_phy
Third body concentration	C_M	(molecular moist air) cm^{-3}	Calculated from density
Water vapor concentration	C_H20	Molecules cm^{-3}	Calculated from qvapor

```
#EQUATIONS { racm-mim }
{001} NO2+hv=O3P+NO : j(Pj_no2) ;
{002} O3+hv=O1D{+O2} : j(Pj_o31d) ;
…
{242} MACP+HO2=MAHP : ARR2( 1.82e-13 , -1300.0, TEMP ) ;
{243} MACP+MACP=HACE+MGLY+0.5 HCHO+0.5 CO+HO2 : 2.00e-12 ;
{244} MSACP+NO2=MPAN : TROE( 9.70e-29 , 5.6 , 9.30e-12 , 1.5 , TEMP, C_M) ;
…
```

Example File 1: Excerpt from the KPP equation (.eqn) file for the RACM-MIM (Geiger et al. 2003) mechanism.

Photolysis rates, temperatures, third body concentrations, and water vapor concentrations are passed down from the WRF-Chem KPP interface routines. Photolysis rates are stored pointwise in a 1-D array and addressed by pointers defined in the automatically generated interface routine. For example, the NO_2 photolysis rate ph_no2 in the Registry. EM CHEM becomes j(pj_no2) in the KPP equation file (see example in Example File 1). Additional variables (e.g. user calculated N_2O_5 hydrolysis rates) can be passed down by modifying .inc files in the WRFV3/chem/KPP/inc directory.

6.10 Adapting additional KPP integrators for WKC

As previously mentioned, only Rosenbrock type solvers are currently available for use with the WKC. Introducing additional integrators which come with KPP into WRF-Chem is rather straight forward, but the process can be very time consuming. The integrator files which come with KPP are located in the directory chem/KPP/kpp/kpp2.1/int. Integrators which have been adapted for WRF-Chem are located in a subdirectory of chem/KPP/kpp/kpp2.1/int named WRF_Conform. The methodology for adapting an additional solver for WRF-Chem is as follows:

- Copy the .f90 and the .def file to the WRF_Conform directory
- Add KPP ROOT as a prefix to the names of the subroutines in all subroutine and end subroutine statements
- Change the arguments in the SUBROUTINE (KPP_ROOT_)INTEGRATE statements to match the calling routine (see the existing integrator routines for an example)

Remove all the USE statements in which non-constant data are used. Instead pass down the data in the subroutine statements. And be aware that, depending on the chosen solver, there may be additional required steps that have not been mentioned above.

Chapter 7: Summary

Table of Contents

7.1 Summary

Presented in this User's Guide is version 3.5 of the WRF-Chem model. This guide is not intended to be an exhaustive report about all that is needed to set up and use the WRF-Chem model. While it does attempt to provide the latest and most accurate information about the configuration and running of the WRF-Chem model, errors or incomplete information may have been unintentionally presented. Also, due to the complexity of the model and the diverse needs of each user, there may be insufficient information for your particular research or operational application. If a user has questions regarding the model that this document fails to answer, the one should contact the WRF-Chem help desk at wrfchemhelp.gsd@noaa.gov, or explore the WRF community forum and see if the user community can povide an answer.

As was stated in beginning chapters, you will need to consider your needs and/or requirements for the domain of interest before beginning the simulation. This includes, but is not limited to the available meteorological and anthropogenic-emissions data sets. Also, the WRF model, and likewise the WRF-Chem model, is being continuously updated. Therefore, you are advised to stay involved in the WRF-Chem user community to be made aware of any and all updates to or issues with the code.

All WRF-Chem users are also advised to link their web browser to the WRF-Chem user group web page (http://www.wrf-model.org/WG11) and periodically scan the pages for changes and/or updates to the model. These web pages contain answers to frequently asked questions, or FAQ's. So this is a good place to start when you have a question regarding the setup, use, or performance of the WRF-Chem model. Finally, this web page contains the most up to date list of relevant publications regarding the WRF-Chem model. When presenting, or publishing results from studies using the WRF-Chem model, it is requested that you cite the Grell et al. (2005) and Fast et al. (2006) manuscripts provided in the relevant publications section of this chapter. For any application that uses the indirect effect, please also cite Gustafson et al. (2007). And likewise, when using other significant features in the WRF-Chem model, the user should examine the reference list on the WRF-Chem web page and cite the developer's paper(s) (http://ruc.noaa.gov/wrf/WG11/References/WRF-Chem.references.htm). A more detailed model description with a series of papers is in the works and may appear in a new journal that is intended for model description papers only.

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Appendix A : WRF-Chem Quick Start Guide

1. Compiling WRF-Chem and the emission converter

a. Download the WRF and then the WRF-Chem from the NCAR web site http://www.mmm.ucar.edu/wrf/users/download/get_sources.htm

b. Set the environmental variables
   i. setenv WRF_CHEM 1
   ii. setenv EM_CORE 1
   iii. setenv FLEX_LIB_DIR /usr/lib (optional)
   iv. setenv WRF_KPP 1 (optional)
   v. setenv YACC '/usr/bin/yacc –d' (optional)

c. Compile WRF-Chem using the command:
   compile em_real >& compile.log

d. Compile convert_emiss using the command:
   compile emi_conv >& emcompile.log

2. Running WRF-Chem with the chemistry turned off

a. Decide which emissions preprocessor you will need to run (step 3 or step 6, see also section 2 in the WRF-Chem User's Guide). This is important, since step 6 requires the user to select a polar stereographic projection for the forecast domain.

b. Produce meteorological input files (wrfinput_d01 and wrfbdy_d01) for the domain of your choice (save these, they will be needed later). Use the WPS to do this. Be sure to choose the map projection based upon your desired emissions data set.

c. First run a meteorology-only simulation to verify the domain you want is functioning correctly, the code has compiled properly, and no issues exist from the meteorological part of the model (set chem_opt=0 in the namelist).

   i. Modify the namlist.input file (to fit your needs and be sure to set chem_opt=0)

   ii. Run real.exe to produce a wrfinput and wrfbdy file

   iii. Run wrf.exe to produce a forecast

iv. Check the resulting output files to verify your forecast results

3. Producing an emissions-input file for your forecast domain using the global RETRO/EDGAR emissions data set available from the ESRL FTP site

a. Get the latest version of the prep_chem_sources tar files from the ESRL web site, including the documentation ftp://aftp.fsl.noaa.gov/divisions/taq/global_emissions

b. Compile prep_chem_sources following the instructions in the README file

c. Modify the prep_sources_chem.inp file for correct domain, and choice of input data

d. Run prep_sources_chem to generate emissions data file

e. From your WRF-Chem run directory, link output files (e.g., WRF-2008-07-15 files) from prep_sources_chem_cptec_wrf
   i. ln –sf ../../../Prep_sources_chem_cptec_wrf/WRF-2008-07-15-000000-g1-gocartBG.bin wrf_gocart_backg
   ii. ln –sf ../../../Prep_sources_chem_cptec_wrf/WRF-2008-07-15-000000-g1-ab.bin emissopt3_d01
   iii. ln –sf ../../../Prep_sources_chem_cptec_wrf/WRF-2008-07-15-000000-g1-bb.bin emissfire_d01
   iv. ln –sf ../../../Prep_sources_chem_cptec_wrf/WRF-2008-07-15-000000-g1-volc.bin volc_d01

f. Edit your namelist.input to reflect the switch to global-emissions data and run convert_emiss.exe. Typically this will require a change to the update interval, the emissions option and possibly the vertical dimension for the emissions. For example, the global data is updated on a monthly basis and is surface data only. So for a typical simulation of a couple of days the emissions data will not be updated (auxiliary input port time intervals are set to a very large number of seconds) and the name list modified for surface only emissions (kemit =1). In addition, the RETRO/EDGAR emissions are for just a few emitted species and the emiss_opt=5 is most often used for this data set.

g. Run the convert_emiss program. It is acceptable if the program was compiled with the distributed memory (dmpar only) as it will run with one or multiple processors. The WRF input files that should be generated are: wrfinput_d01 (2a), the files from set (e.) above, and your WRF namelist.input.

h. Check whether the program successfully produced the emissions input (wrfchemi_d01 or wrfchemv_d01, wrffirechemi_d01 and wrfchemi_gocart_bg_d01). These should all be netcdf files if you specified that I/O form in your namelist.input file and so you can check the data with utilities like ncview or ncbrowse.

4. Running WRF-Chem (multiple processors may be necessary due to large memory requirements, depending on your domain size)

a. Modify the name list to suit your needs (check Chapter 3 of the User's Guide to select your name list options, and Chapter 4 as guidance for some typical setups)

b. Run real.exe to produce the wrfinput file that includes chemistry. Check the output using ncview or ncbrowse or similar programs

c. Confirm that you have the emissions files for the simulation in the run directory. If necessary, rename your emissions files (or link them) to the files wrfchemi_00z_d01 and/or wrfchemi_12z_d01 (for io_style_emissions=1)

d. Run wrf.exe.

e. Inspect the model results to make sure your namelist.input settings were correct

5. Visualizing the output can be done with various packages, including ncview, NCL, RIP, ncbrowse, GRADS

The output from the WRF-Chem model is a standard WRF output netCDF data file. Therefore, your favorite netCDF data file viewer can be used to examine results. For example, the ncview program will allow the users to quickly view the model output.

Additional Options

6. Using the NEI data set for domains located over the USA

a. Download the emiss_v03.F program and the emission data from the ESRL anonymous ftp site, or through your web browser by setting the URL to: ftp://aftp.fsl.noaa.gov/divisions/taq/emissions_data_2005

b. Modify the emiss_v03.F program file to correspond to your domain setup (see also section 2 of the User's Guide).

c. Compile emiss_v03.F
   i. There are examples provided at the beginning of the program like for the case when using pgi, the suggested compile commands would be
   > pgf90 –w –byteswapio –Mfree –Mlfs –o emiss_v03.exe emiss_v03.F

d. Run emiss_v03.exe to produce an emissions file for a domain located over the contiguous states. Two binary data files will be produced called wrfem_00to12Z and wrfem_12to24Z. You can re-name them after the simulation run, or edit the emiss_v03.F to have the program produce a name that suits your liking.

e. Move the binary output files with the prefix "wrfem" from where you have run the program to WRFV3/run for use later on by the convert_emiss.exe program.

f. Go to the test/em_real directory and link the binary emissions files from (3e) to the files that are used by the WRF-Chem code
   i. ln –sf wrfem_00to12Z wrfem_00to12z_d01
   ii. ln –sf wrfem_12to24Z wrfem_12to24z_d01

g. Modify the namelist.input file to have the correct update time interval (auxinput5_interval_m for anthropogenic emissions.) for each auxiliary input. Default output time interval from emiss_v03 is 3600 seconds. You should also set the correct emission input option (emiss_opt=3 for NEI emissions) for the anthropogenic emissions and your choice of chem_opt (see section 3.2 of the User's Guide). In addition, the NEI emissions include smoke stack emissions so the input data will have a vertical dimension set with the kemit option.

h. Run the convert_emiss program. Run this program with one processor only. It is acceptable if the program was compiled with the distributed memory option, but do not run it with more than 1 processor. Required

input files are: wrfinput_d01 (2a), wrfem_00to12z_d01 and/or wrfem_12to24z_d01 (3f), and namelist.input.

i. Check whether the program successfully produced the emissions input (wrfchemi_d01_xxz or wrfchemi_d<domain>_<date>). These are netcdf files, you can check them with ncview or ncbrowse.

7. Special biogenic emissions files

There are four choices in the model for biogenic emissions.

a. The first option is not to use an additional biogenic-emissions input data file (bio_emi_opt= 0). The user could add the biogenic emission to the anthropogenic-emissions data if it is desired. Be sure to do this for every time period in the emissions input data and not just the first time.

b. For the second option (bio_emi_opt= 1), the model calculates the biogenic emissions online using the USGS land-use classification, which is generated by WRF WPS and available for the meteorological and chemical model.

c. For the third option, the user-specifies reference fields for the biogenic emissions, which are then modified online by a subroutine from the Biogenic Emissions Inventory System (BEIS) version 3.14. The land-use for this emissions inventory is obtained from the Biogenic Emissions Landuse Database version 3 (BELD3). The reference fields need to be provided as an additional input data file (wrfbiochemi_d01) for the real.exe program.

d. The final option is the use of MEGAN, which again requires the preparation of reference fields (Appendix C of the User's Guide)

8. Nesting

a. Produce wrfinput files for both domains following Chapter 4 of WRF User's Guide

b. Like the single domain WRF-Chem simulations, it is probably best to make a nested domain weather forecast (Chapter 5 of WRF User's Guide)

c. Generate the emissions files for both domains using the emiss_v03.F program (section 3 of Quick Step Guide, Chapter 2 of the WRF-Chem User's Guide). File names will need to differentiate between the domains (e.g., wrfem_00to12z_d01 and wrfem_00to12z_d02)

d. The convert_emiss.exe program is not currently designed to read the namelist.input file and generate the nested domain emissions files. Therefore, run the conversion program treating the nested domain as if it was actually the mother domain

    i. Follow 3f – 3i to generate wrfchemi_d01 for the coarse domain, move it to a safe place so that they will not be overwritten

    ii. Change the namelist.input file. Moving the nested information to the mother domain column

    iii. Move the met wrfinput_d02 to wrfinput_d01

    iv. Link the output from emisv03 (for the nested domain) to the required filenames (see 3h)

    v. Run convert_emiss.exe

    vi. Move the resulting wrfchemi_d01 to wrfchemi_d02

e. Modify the namelist.input file to set the chemistry namelist variables for the nested domain

9. Boundary conditions from larger scale models

At this time, tools are still under development to provide larger scale data from models other than WRF as boundary and initial conditions to the WRF-Chem simulations. One such utility program that is available from NOAA/ESRL is called wrfchembc. This program currently works with data from the MPI-MATCH and RAQMS global chemistry models.

a. Download the latest version of the code from the ESRL ftp site. For example, the latest code might be named

    ftp://aftp.fsl.noaa.gov/divisions/taq/broken_experimental/wrfchemv2.2_bcond_code_09Apr07.tar

b. Modify the Makefile to use your desired compile options and compile to generate the wrfchembc executable

c. Modify the wrfchembc_namelist.input file to have the correct data directories and species added to the boundary data file (wrfbdy_d01)

d. Run the wrfchembc program after real.exe and before wrf.exe to add the global model data to the lateral boundary data file (wrfbdy_d01)

e. Before running wrf.exe, modify the namelist.input to set have_bcs_chem = .true

f. Make a forecast using wrf.exe and inspect the model results to make sure your namelist.input settings were correct

Another tool for generating chemica lateral boundary conditions is available from NCAR/ACD and is called mozbc. The mozbc utility and is provided to the community at the NCAR/ACD website http://www.acd.ucar.edu/wrf-chem and along with the code the user can obtain MOZART model data for the dates and location of interest. The user is directed to the NCAR/ACD web site for the latest information regarding this utility.

Appendix B: Using prep_chem_sources V1.3

Source Distribution Layout

The top level of the source code distribution contains the following subdirectories:

bin -- Scripts for maintenance, execution, compilation
src -- Source codes
aux_src -- Auxiliary codes

Third-Party Software Requirements

JPEG distribution release 6b(libjpeg.a). You may download the software from http://www.hdfgroup.org/release4/obtain.html
ZLIB 1.2.1(libz.a) or later distribution. You may download the software from the http://www.gzip.org/ site.
HDF5 1.8 (libmfhdf.a, libdf.a) or later distribution. You may download the software from http://www.hdfgroup.org/downloads/index.html
NetCDF 4.0.1 (libnetcdf.a). You may download the software from http://www.unidata.ucar.edu/downloads/netcdf/netcdf-4_0_1/index.jsp

Configuring/Installing HDF5

When compiling PREP-CHEM-SRC codes on a Linux system using the PGI (Intel) compiler, make sure the netCDF and HDF library has been installed using the same PGI (Intel) compiler. For example, you will probably need to con figure the HDF library build using command lines like

```
./configure --prefix=path_hdf5    \
--with-jpeg=path_jpeg \
                --with-zlib=path_zlib \
                --disable-netcdf
make && make install
```

Configuring/Installing the prep_chem_sources code

To compile the version 1.3 code one needs to change directory to the bin/build directory

cd bin/build

and verify the compiler and library path settings in the include.opt.<your compiler> make option file. The user should set similar library paths and compile options (e.g., byte swapping) as used for the WRF-Chem code compilation otherwise the code might not compile or the binary intermediate output will be unreadable by the WRF-Chem convert

program. Then, once the make option include file is configured for your computer system, the make command is issued with the compiler option (e.g., Intel, PGI) and the chemistry option (ie., RADM_WRF_FIM) listed in the command line

make OPT=opt.pgi CHEM=RADM_WRF_FIM

Using PREP-CHEM-SRC-1.3 with WRF-Chem V3.5

To run the prep_chem_sources executable one must first edit the name list input fields. Most of the settings are like the previous versions with the exception of the map projection settings. But fortunately the map projection settings correspond to the map projection settings used in the WPS input file namelist.wps. That is:

NINEST=i_parent_start,
NJNEST=j_parent_start,
POLELAT=ref_lat,
POLELON=ref_lon,
STDLAT1=truelat1,
STDLAT2=truelat2.

The prep_chem_sources settings CENTLAT and CENTLON are not used for WRF, but are most often the latitude and longitude of the central grid point for your domain.

After setting the prep_chem_sources name list one can run the PREP-CHEM-SRC executable (e.g., prep_chem_sources_RADM_WRF_FIM.exe) for each day to produce the intermediate data files. These files are the anthropogenic- and biogenic-emissions file (ending with -ab.bin), the biomass burning-emissions file (ending with -bb.bin), and the GOCART background data (ending with -gocartBG.bin).

Once the prep_chem_sources executable has been run, the methodology for converting the binary intermediate files is outlined in section 3.2 of this User's Guide, but it will be quickly recapped here. For each day that you are going to use the global emissions data, you need to run the convert_emissions program. This program will also need a wrfinput data file for the desired date as well. So to begin, one can run the real.exe with chem_opt=0 and start and end time set to your year, month, day, and start hour generate a wrfinput_d01 file. Then the output from prep_chem_sources is linked to the WRF running directory (e.g., WRFV3/test/em_real) with commands similar to the following:

```
ln -sf WRF-2011-07-14-000000-g1-gocartBG.bin ../../WRFV3/test/em_real/wrf_gocart_backg
ln -sf WRF-2011-07-14-000000-g1-ab.bin       ../../WRFV3/test/em_real/emissopt3_d01
ln -sf WRF-2011-07-14-000000-g1-bb.bin       ../../WRFV3/test/em_real/emissfire_d01
ln -sf WRF-2011-07-14-000000-g1-volc.bin     ../../WRFV3/test/em_real/volc_d01
```

And then before one can run the convert emissions program convert_emiss (convert_emiss.exe) the namelist.input settings for the chemistry needs to be turned back on (e.g., chem_opt=301). Be sure to double check your other namelist settings as well or you might not get the desired data files.

```
&time_control
 io_form_auxinput5               = 2
 io_form_auxinput6               = 2
 io_form_auxinput7               = 2
 io_form_auxinput8               = 2
 io_form_auxinput12              = 2,
 io_form_auxinput13              = 0,
 auxinput6_inname               = 'wrfbiochemi_d01',
 auxinput7_inname               = 'wrffirechemi_d<domain>',
 auxinput8_inname               = 'wrfchemi_gocart_bg_d<domain>',
 auxinput12_inname               = 'wrf_chem_input',
 auxinput13_inname               = 'wrfchemv_d<domain>'
 auxinput5_interval_m            = 1440,1440
 auxinput7_interval_m            = 1440,1440
 auxinput8_interval_m            = 1440,1440
 auxinput13_interval_m            = 1440,1440
 frames_per_auxinput6            = 1,1
 frames_per_auxinput7            = 1,1
 frames_per_auxinput8            = 1,1
 frames_per_auxinput13             = 1,1
/

&chem
 kemit                           = 1,
 chem_opt                        = 301,    2,
 io_style_emissions              = 2,
 emiss_inpt_opt                  = 1,       1,
 emiss_opt                       = 5,       5,
 emiss_opt_vol                   = 0,       1,
 biomass_burn_opt                = 1,       1,
 plumerisefire_frq               = 120,     120
```

And when complete and the data files are verified you can rename output to include the date if so necessary

```
mv wrfchemi_d01 wrfchemi_d01_{$year}-$mo-${da}_00:00:00
```

Appendix C: Using MEGAN with WRF-Chem

Introduction

The University Corporation for Atmospheric Research (UCAR) provides Fortran source code files to create MEGAN (Model of Emissions and Gases from Nature) biogenic emission data for importing into WRF-Chem. MEGAN is a global emissions dataset, at one-kilometer spatial resolution, compiled for 2003. A users guide and descriptions of the data set are provided at http://bai.acd.ucar.edu/Megan/.

The MEGAN toolkit for WRF-Chem preprocesses the MEGAN data set, and creates wrfbiochem_d0x (x = domain number) input files for ingestion into WRF-Chem at model run time.

The following instructions assume that real.exe and wrf.exe have been compiled normally and that an initial meteorology only wrfinput_d0x file(s) have been created post WPS. These instructions also assume you are using the provided 2003 MEGAN data files. The tar file from UCAR includes a helpful readme file which expands on the instructions below.

Compiling

1) Download the MEGAN preprocessor Fortran source code and data set from http://www.acd.ucar.edu/wrf-chem/. You will be asked to register some contact details – subsequently click the "bio-emiss" button on the user registration page to download the MEGAN Fortran source code, makefile and MEGAN data input files. The files can be downloaded to a directory of your choice – note that the process of using MEGAN needs to access the WRF run directory and the wrfinput_d01 file during MEGAN data preprocessing.

2) un-tar the files downloaded in the MEGAN directory by issuing the commands:

```
>tar –xvf bio_emiss.tar
```

   This creates two other tar files, un-compress and un-tar these files:

```
>tar –xvf megan_bio_emiss.tar
>tar –zxvf megan.data.tar.gz
```

3) Ensure the correct environment variables for your Fortran compiler and netCDF libraries are set correctly by editing the make_util script file if necessary

4) Compile the MEGAN source code in the MEGAN directory by issuing the command:

```
>make_util megan_bio_emiss
```

   This will create the executable file – megan_bio_emiss

Preprocessing

5) Run real.exe for meteorology only to produce files that will contain WRF headers. This step is similar for all emissions input creation. This step will create a file named wrfinput_d01 that does not contain any input for MEGAN. The following MEGAN pre-processing steps utilize the wrfinput_d01for geographical and temporal parameters necessary for the production of wrfbiochem_d0x files.

6) Adjust the text file; megan_bio_emiss.inp, for:
   1. domains – the number of domains used in your WRF model
   2. start_lai_month - this should be set as the month before the month in which your WRF run is set to start
   3. end_lai_month – this should be set as the month in which your WRF run is set to end
   4. wrf_dir – the directory where the associated wrfinput_d01 resides, and
   5. megan_dir – the directory in which the MEGAN data files exist

   Note – lai (or leaf area index) parameter data files are provided in the MEGAN preprocessing download – one file exists for each month.

7) Create MEGAN bioegenic-emissions data for your domain and time frame by issuing the command:

   >megan_bio_emiss < megan_bio_emiss.inp > megan_bio_emiss.log

   Note – this serial process can take some time depending on a range of factors (perhaps 10 minutes for a lambert conformal projection).

   Check megan_bio_emiss.log for any errors or problems.

8) The files created are wrfbiochemi_d0x files which should be copied (or linked) into the associated WRF run directory.

   You might review the wrfbiochemi_d0x files with ncview to ensure the correct geographical bounds have been applied and that the MEGAN data sets are included.

   Note – the MEGAN data elements in the wrfbiochemi_d0x files are:
   - MSEBIO_ISOP amount of isoprene (mol km^{-2} hr^{-1})
   - PFTP_BT percentage of broad leaf
   - PFTP_NT percentage of needle leaf
   - PFTP_SB percentage of shrubs
   - PFTP_HB percentage of herbaceous biota
   - MLAI monthly leaf area index
   - MTSA monthly air temperature (K), and
   - MSWDOWN monthly download short wave radiation (W m^{-2})

Running WRF-Chem with MEGAN

9) To create the WRF-Chem boundary and combined emission files, run real.exe like normal in a directory that contains the files wrfbiochemi_d0x (from step 8), but with bio_emiss_opt=3 and ne_area set to a value equal to or greater than the total chemical species used. With bio_emiss_opt=3, real.exe will create wrfinput_d01 containing inputs required for running MEGAN online.

   Note - wrfbiochemi_d01 and wrfinput_d01 will also include variables for running BEIS3.14, but the values for BEIS variables will all be all zero; you'll need to create a different wrfbiochemi_d01 file if you want to use bio_emiss_opt=2.

10) Now, you can run wrf.exe with MEGAN emissions calculated online using bio_emiss_opt=3 and input through the auxiliary input ports.

    Note – the process of using wrf_biochemi_d0x files in WRF-Chem model runs will depend on how many WRF-Chem domains you have in mind. For a single domain, one wrf_biochemi_d01 file will be produced. Using more than one domain (therefore wrf_biochemi_d0x files, where x = 1, 2 to the maximum domain number) involves careful application of model processes as documented elsewhere in this manual. It can be complex using MEGAN data files for 2-way or 1-way (n-down or 2-way with feedback to the coarse domain switched off) nesting WRF-Chem processes. However, assuming the wrfinput_d0x files are setup correctly before preprocessing MEGAN data files, the wrf_biochemi_d0x files will match the geographical extent of the wrfinput_d0x files. This is slightly less complicated than the process needed to compile the baseline wrfchemi_d0x files.

Appendix D: Using MOZART with WRF-Chem

Introduction

The National Center for Atmospheric Research (NCAR) provides Fortran source code to prepare additional data files to support the MOZART (Model for OZone And Related chemical Tracers) gas-phase chemistry scheme in WRF-Chem. These files are needed to update WRF-Chem parameters suitable for MOZART. MOZART gas-phase chemistry can be combined with GOCART aerosol treatment – known as MOZCART in this manual.

When setting up WRF-Chem to use MOZART/MOZCART, the user should select the FTUV photolysis option (phot_opt=3) in the namelist.input file. NCAR advises the FTUV code has been updated to read in O_3 and O_2 climatological atmospheric column values rather than fixed values. This requires an additional input file for each domain – exo_coldens_d<nn> (nn = domain number). The exo_colden utility (for single CPU) reads WRF-and MOZART-input files and produces netCDF files for each WRF domain.

When using dry deposition in WRF-Chem (gas_drydep_opt=1) combined with MOZART (and MOZCART) scheme in WRF-Chem, NCAR advises that an additional file for each domain is required – wrf_season_wes_usgs_d<nn> (nn = domain number). The wesely utility (for single CPU) reads WRF and MOZART input files and produces netCDF files for each WRF domain.

The tar file from NCAR includes a helpful readme file which expands on the instructions below. NCAR provides some information at http://www.acd.ucar.edu/wrf-chem/MOZCART_UsersGuide.pdf which provides a table mapping MOZART emissions species to EPA/NEI species as well as contact details at NCAR for further support.

Compiling

1) Download the MOZART preprocessor Fortran source code from http://www.acd.ucar.edu/wrf-chem/. You will be asked to register some contact details – subsequently click the "preprocessor" button on the user registration page to download the MOZART Fortran source code, makefile, and MOZART-data input files. The files can be downloaded to a directory of your choice – note that the process of using MOZART needs to access the WRF run directory and the wrfinput_d01 file during MOZART data preprocessing.

2) Un-tar the files downloaded in a directory of your choice by issuing the commands:
   >tar –xvf wes_coldens.tar

3) Compile the MOZART source code by issuing the commands:
   >make_util wesely

>make_util exo_coldens

This will create the executable files – wesely and exo_coldens.

Preprocessing

4) The wesely program reads WRF wrfinput_d<nn> files and a MOZART-data file containing dry emission parameters - season_wes_usgs.nc (found in the tar file above). Adjust the text file wesely.inp for:
   1. domains – the number of domains used in your WRF model
   2. pft_flnm – season_wes_usgs.nc
   3. wrf_dir – the directory where the associated wrfinput_d<nn> resides, and
   4. pft_dir – the directory in which the MOZART data file exists

5) To create the wesely data files for MOZART, issue the command:
   >wesely < wesely.inp > wesely.out

   This creates a file for each domain wrf_season_wes_usgs_d<nn> which should be copied to the WRF run directory for use in WRF-Chem MOZART/MOZCART model runs.

6) The exo_colden program reads WRF wrfinput_d<nn> files and a MOZART data file exo_coldens.nc (found in the tar file above). Adjust the text file exo_coldens.inp for:
   A. domains – the number of domains used in your WRF model
   B. exo_flnm – exo_coldens.nc
   C. wrf_dir – the directory where the associated wrfinput_d<nn> resides, and
   D. exo_dir – the directory in which the MOZART data file exists

7) To create the exo_coldens data files for MOZART, issue the command:
   >exo_coldens < exo_coldens.inp > exo_coldens.out

   This creates a file for each domain exo_coldens_d<nn> which should be copied to the WRF run directory for use in WRF-Chem MOZART/MOZCART model runs.

Running WRF-Chem with MOZART (MOZCART)

8) Selecting the MOZART/MOZCART settings in the namelist.input of the WRF-Chem run directory (chem_opt and emiss_opt) will switch on the ingestion of the files noted above into WRF-Chem.

Appendix E: Using the Lightning-NOx Parameterization in WRF-Chem

The WRF-Chem model has a parameterization able to provide an estimate of the lightning-generated nitrogen oxides production (LNOx). The LNOx parameterization is based on the Price and Rind (1992, hereafter PR92) schemes with modifications based on Barth et al. (2012) and Wong et al. (2013). To determine LNOx, the lightning flash rate, the location (both horizontally and vertically), and the amount of NO produced per flash must be estimated. The lightning flash rate parameterization is located in the physics directory using module_lightning_driver.F, which is called from dyn_em/solve_em.F. The location and production of NO per flash parameterization is located in the chem directory using module_lightning_ nox_driver.F, which is called from emissions_driver.F. The parameterization of lightning-generated NOx is valid for both parameterized convection and resolved convection, but different parameters may be used. Details on the parameters used in the namelist.input file are explained next.

Physics section:

To turn on the lightning flash rate parameterization in WRF, set the *physics* namelist option lightning option to one of the following values:

lightning_option	**Description**
1	PR92 based on maximum *w*; distributes flashes within dBZ > 20 For convection-resolved resolutions with microphysics turned on for reflectivity calculations.
2	PR92 based on 20 dBZ cloud top; distributes flashes within dBZ > 20 For convection-resolved resolutions with microphysics turned on for reflectivity calculations.
11	PR92 based on level of neutral buoyancy obtained from convective parameterization For convection-parameterized resolution using either GD or G3 cu physics options. Adjusted by areal ratio relative to dx=36 km (Wong et al., 2013), intended for use at 10 < dx < 50 km.

Setting the lightning option will produce four new 2D arrays: ic_flashrate, cg_flashrate both with units number per second, and ic_flashcount, cg_flashcount with units number of flashes, where ic and cg represent intra-cloud and cloud-to-ground, respectively. The ic_flashrate and cg_flashrate arrays are instantaneous output that can be used to diagnose the lightning flashrate and LNOx parameterizations. The arrays ic_flashcount, cg_flashcount accumulate the number of flashes during the simulation. To find the number of flashes between output times, simply subtract the flashcount array from the previous output time from the current output time to get number of flashes per dt (where

dt = time between output files).

Set the *physics* namelist option iccg_method to control the IC:CG ratio:

iccg_method	Description
0	Default method depending on lightning_option, currently all options use iccg_method=2 by default.
1	Constant everywhere, set with namelist options iccg_prescribed_num (numerator) and iccg_prescribed_den (denominator).
2	Coarsely prescribed 1995–1999 NLDN/OTD climatology based on Boccippio et al. (2001).
3	Parameterization by Price and Rind (1993) based on cold-cloud depth.
4	Gridded input via arrays iccg_in_num (numerator) and iccg_in_den (denominator) from wrfinput for monthly mapped ratios.

Additional namelist settings in the *physics* section are available for more detailed control of the parameterization:

Namelist Option	Description
iccg_prescribed_num	Prescribes numerator of IC:CG ratio. Used by iccg method=1,4 Default = 0
iccg_prescribed_den	Prescribes denominator of IC:CG ratio. Used by iccg method=1,4 Default = 1
iccg_in_num	Gridded array from the wrfinput file for monthly mapped IC:CG ratios. iccg_in_num is the numerator of the ratio. Gridpoints with iccg_in_num=0 and iccg_in_den=0 values use ratio defined by iccg_prescribed_num and iccg_prescribed_den. See more information below.
iccg_in_den	Gridded array from the wrfinput file for monthly mapped IC:CG ratios. iccg_in_den is the denominator of the ratio. Gridpoints with iccg_in_num=0 and iccg_in_den=0 values use ratio defined by iccg_prescribed_num and iccg_prescribed_den. See more information below.
lightning dt	Time interval (seconds) for calling lightning parameterization. Default uses model time step.
lightning start seconds	Start time for calling lightning parameterization. Recommend at least 10 minutes for spin-up.

flashrate factor	Factor to adjust the predicted number of flashes. Recommend 1.0 for lightning option=11 between dx=10 and 50 km. Manual tuning recommended for all other options independent for each nest.
cellcount method	Method for counting storm cells. Used by CRM options (lightning options=1,2). 0 = model determines method used. 1 = tile-wide, appropriate for large domains 2 = domain-wide, appropriate for single-storm domains
cldtop_adjustment	Adjustment from LNB in km. Used by lightning option =11. Default is 0, but recommends 2 km.

Gridded data of the IC:CG ratios written in the form of a ratio numerator and denominator (iccg_in_num and iccg_in_den) can be read from the wrfinput file to prescribe the IC to CG flash ratio. To get the gridded data into the wrfinput file, the user needs to interpolate the IC:CG ratio dataset to the WRF grid as a pre-processing step. The user also needs to provide his/her own dataset.

Chemistry section:

To emit LNOx, in the form of nitrogen oxide (NO), set the *chem* namelist option lnox_opt to one of the following values:

lnox_option	Description
1	Combined IC+CG single-mode vertical distributions (Ott et al., 2010). Outputs passive tracer array in addition to the NO source.
2	Separate IC, CG vertical distributions following DeCaria et al. (2000). In addition to providing a source to NO, outputs two passive tracer arrays lnox_ic and lnox_cg.

Additional *chem* namelist settings are available for more detailed control of the parameterizations:

Namelist Option	Description
N_IC	Moles of NO emitted per IC flash. For lnox opt=1, the total number of moles NO per flash is the weighted average based on the calculated IC:CG ratio of N_IC and N_CG. Default is 500 moles.
N_CG	Moles of NO emitted per CG flash. For lnox opt=1, the total

	number of moles NO per flash is the weighted average based on the calculated IC:CG ratio of N_IC and N_CG. Default is 500 moles.
lnox_passive	Set to .true. to emit passive tracers only. Set to .false. to emit both NO and passive tracer. Default = .false.
ltng_temp_upper	Temperature (C) of upper peak of LNOx vertical distribution for IC lightning (used by lnox opt=2).
ltng_temp_lower	Temperatures (C) of lower peak of LNOx vertical distribution for both IC and CG lightning (used by lnox opt=2).

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